ESSENTIAL SPECTRAL EQUIVALENCE VIA MULTIPLE STEP PRECONDITIONING AND APPLICATIONS TO ILL CONDITIONED TOEPLITZ MATRICES

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Abstract. In this note, we study the fast solution of Toeplitz linear systems with coefficient matrix $T_n(f)$, where the generating function $f$ is nonnegative and has a unique zero at zero of any real positive order $\theta$. As preconditioner we choose a matrix $\tau_n(f)$ belonging to the so-called $\tau$ algebra, which is diagonalized by the sine transform associated to the discrete Laplacian. In previous works, the spectral equivalence of the matrix sequences $\{\tau_n(f)\}_n$ and $\{T_n(f)\}_n$ was proven under the assumption that the order of the zero is equal to 2: in other words the preconditioned matrix sequence $\{\tau_n^{-1}(f)T_n(f)\}_n$ has eigenvalues, which are uniformly away from zero and from infinity. Here we prove a generalization of the above result when $\theta < 2$. Furthermore, by making use of multiple step preconditioning, we show that the matrix sequences $\{\tau_n(f)\}_n$ and $\{T_n(f)\}_n$ are essentially spectrally equivalent for every $\theta > 2$, i.e., for every $\theta > 2$, there exist $m_\theta$ and a positive interval $[\alpha_\theta, \beta_\theta]$ such that all the eigenvalues of $\{\tau_n^{-1}(f)T_n(f)\}_n$ belong to this interval, except at most $m_\theta$ outliers larger than $\beta_\theta$. Such a nice property, already known only when $\theta$ is an even positive integer greater than 2, is coupled with the fact that the preconditioned sequence has an eigenvalue cluster at one, so that the convergence rate of the associated preconditioned conjugate gradient method is optimal. As a conclusion we discuss possible generalizations and we present selected numerical experiments.

Key words. Toeplitz, preconditioning, $\tau$ matrices, spectral analysis, PCG method.

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1. Introduction. Our goal is to design and analyze a preconditioning technique for the fast solution of a Toeplitz system with $n \times n$ coefficient matrix $T_n(f)$, where $f$ is a given function having a unique zero at zero of positive order $\theta$: the entry $(j,k)$, $1 \leq j,k \leq n$, of the matrix $T_n(f)$ is the $l$-th Fourier coefficient of $f$ with $l = j - k$ and

$$a_l = \frac{1}{2\pi} \int_0^{2\pi} f(t)e^{-ilt} dt.$$ 

The preconditioner is chosen in the so-called $\tau$ algebra which is the set of all real symmetric matrices diagonalized by the sine transform associated to the discrete Laplacian (see (2.2)): the preconditioner is chosen to have as eigenvalues a uniform sampling of the symbol $f$ and is denoted by $\tau_n(f)$.

We study the spectrum of the matrix sequences $\{A_n\}_n$ with $A_n = \tau_n^{-1}(f)T_n(f)$ with the goal of localizing the eigenvalues and understanding the asymptotic behavior. We recall that the study of such a matrix sequence gives precise information on the convergence speed of the related preconditioned Conjugate Gradient (PCG) method and the associated preconditioning strategy can be used in connection with multigrid schemes: see [2] for the use of fast Toeplitz preconditioning in the context of a multigrid method for a Galerkin isogeometric analysis approximation to the solution.

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of elliptic partial differential equations. Furthermore, the analysis of the sequence \( \{A_n\}_n \) can be helpful in the development of new approaches as the Jacobi-Davidson method in the context of eigenvalue problems.

The problem of understanding the spectrum of \( \{A_n\}_n \) has been extensively studied in the literature, see for example [12], [5] and references therein, when the generating function has zeros of even multiplicity. Here, to the best of our knowledge, it is the first time that the general case is considered. For the sake of simplicity, we restrict our attention to the case where \( f \) has a unique zero at zero with positive order \( \theta \): it is worthwhile observing that in such a context the band Toeplitz preconditioning cannot lead to spectrally equivalent or essentially spectrally equivalent sequences, just because a nonnegative trigonometric polynomial cannot have zeros of non even order (see [16] for a discussion on the subject).

The spectral relations between Toeplitz and \( \tau \) matrices have been analyzed by many researchers. Specifically, the spectral properties of this algebra are investigated in [3] and its approximation features, in connection with Toeplitz structures, are treated in [4]. In [7], [6], [10] several \( \tau \) preconditioning techniques are studied, while in [8] the spectral properties of \( \tau \) preconditioned matrices are considered in detail.

In the quoted literature, in order to perform a theoretical analysis, the authors assumed that the generating function has zeros of even orders. The novel contribution of this work relies on the relaxation of this assumption. Precisely, we study the spectral properties of the matrix sequence \( \{A_n\}_n \), by dividing the analysis into two steps: first we consider the case where the order of the zero is \( \theta \in (0, 2] \) and then, by using a multiple step preconditioning, we consider the case \( \theta > 2 \), which is somehow reduced to the first case.

The paper is organized as follows. §2 contains the necessary preliminary definitions: in particular we define the \( \tau \) algebra, the preconditioner, and the notion of (essential) spectral equivalence. In §3 we briefly describe the tools we use i.e., a special block Toeplitz operator and the multiple step preconditioning. The main theoretical statements of this paper are presented and proved in §4 and concern the assumptions which leads to the (essential) spectral equivalence between ill conditioned Toeplitz sequences and the associated \( \tau \) preconditioners. In §5 we report and critically discuss various numerical experiments, while Section 6 is devoted to concluding remarks and to potential future extensions.

2. Preliminaries. Let \( f \) be a nonnegative even function having, for simplicity, a single zero at the point \( x_0 = 0 \) of order \( \theta \in \mathbb{R}^+ \), where \( \mathbb{R}^+ \) is the set of positive real numbers, and let \( \{T_n(f)\}_n \) be the related Toeplitz matrix sequence. Then, the \( \tau \) sequence \( \{P_n\}_n \) constructed as

\[
P_n = \tau_n(f) = S_n \text{diag}(f(w^{[n]})) S_n
\]

is considered as a preconditioning sequence for \( \{T_n(f)\}_n \); here \( w^{[n]} \) is the \( n \) dimensional vector with entries \( w_i^{[n]} = \frac{\pi i}{n+1}, i = 1, \ldots, n \), \( S_n \) is the sine-transform matrix defined as

\[
(S_n)_{ij} = \sqrt{\frac{2}{n+1}} \left( \sin(jw_i^{[n]}) \right)_{i,j=1}^n,
\]

and \( \text{diag}(f(w^{[n]})) \) is the diagonal matrix having as diagonal entries, the sampling of the values of \( f \) on the specific discretization \( w^{[n]} \). Obviously, \( P_n \) is always positive definite and the same holds true whenever the zero (or zeros) of the generating function
does not coincide with the discretization points \( w^{(n)} \). Under this assumption, the developed theory of the next section holds unaltered. We mention that the \( \tau \) matrices constructed in this way are not the “Frobenius optimal” \( \tau \) preconditioners \([4]\): they coincide with the “natural” \( \tau \) preconditioner only if \( f \) is a trigonometric polynomial (see e.g. \([18]\)).

The main goal of this work is to show that the sequences of matrices \( \{ P_n = \tau_n(f) \}_n \) and \( \{ T_n(f) \}_n \) are spectrally equivalent whenever the symbol \( f \) has a unique zero at zero of order \( \theta \leq 2 \). Moreover, when \( \theta > 2 \), the essential spectral equivalence between these two sequences of matrices can be proven. The notions of spectral and essential spectral equivalence are reported below.

**Definition 2.1.** Given two sequences of positive definite matrices, \( \{ A_n \}_n \) and \( \{ P_n \}_n \) we say that they are spectrally equivalent iff the spectrum \( \{ \sigma(P_n^{-1}A_n) \}_n \) of \( \{ P_n^{-1}A_n \}_n \) belongs to a positive interval \([\alpha, \beta]\), where \( \alpha, \beta \) are constants independent of \( n \) with \( 0 < \alpha \leq \beta < \infty \). We say that the sequences \( \{ A_n \}_n \) and \( \{ P_n \}_n \) are essentially spectrally equivalent iff \( \{ \sigma(P_n^{-1}A_n) \}_n \) is contained in \([\alpha, \beta]\), with at most a constant number of outliers greater than \( \beta \).

### 3. Tools.

As we have mentioned in the introduction, the theoretical tools that are used in the literature to prove the (essential) spectral equivalence between ill conditioned Toeplitz sequences generated by a symbol having a zero of even order at zero, and proper matrix algebra sequences, cannot be applied in our case. Thus, the main tools for proving our arguments will be results coming from block Toeplitz matrices, properties on Schur complements, the flexibility of the Rayleigh quotient in the min-max, max-min characterizations of eigenvalues of Hermitian matrices, and a general theorem on the multiple step preconditioning. A brief overview of them is presented in the next subsections.

#### 3.1. A special block Toeplitz operator.

Regarding block Toeplitz matrices, we remind that if \( F(t) \) is a \( 2 \times 2 \) matrix-valued function of the form

\[
F(t) = \begin{pmatrix} f_1(t) & f_2(t) \\ f_3(t) & f_4(t) \end{pmatrix},
\]

then, the matrix

\[
B_{2n}(F) = \begin{pmatrix} T_n(f_1) & T_n(f_2) \\ T_n(f_3) & T_n(f_4) \end{pmatrix}
\]

is a block Toeplitz matrix. Note that the resulting structure, and consequently its spectral properties, are quite different from the ones of the scalar and multi-level Toeplitz forms, but there is a strong link with the one-level Toeplitz matrices generated by a matrix-valued function. In fact, there exists a simple permutation \( \Pi \) such that

\[
T_n(F) = \Pi B_{2n}(F) \Pi^T
\]

and hence the spectrum of \( B_{2n}(F) \) coincides with that of \( T_n(F) \). Furthermore, from the analysis in \([11]\), it is known that \( T_n(F) \) (and so \( B_{2n}(F) \)) is positive semidefinite, whenever the generating function \( F \) is positive semidefinite and, in addition, \( T_n(F) \) is positive definite if the minimal eigenvalue of \( F \) is not identically zero; see \([17]\). We will use these properties later on in our main derivations in Theorem \([11]\).
3.2. The multiple step preconditioning. Consider a linear system with a positive definite coefficient matrix $A_n$ and suppose we have a chain of positive definite preconditioners $P_n^{(0)}, \ldots, P_n^{(l)}$ such that $P_n^{(j+1)}$ is an optimal preconditioner for $P_n^{(j)}$ (i.e., we have essential spectral equivalence between the two sequences), $j = 0, \ldots, l-1$, $P_n^{(0)} = A_n$.

Then, a natural approach is to use a PCG at the external level with coefficient matrix $A_n$ and preconditioner $P_n^{(1)}$. Furthermore, for all the auxiliary linear systems involving $P_n^{(1)}$, we use again a PCG method with $P_n^{(2)}$ as preconditioner and so on. Given the optimal convergence rate of all the considered PCG methods, it is easy to see that the global procedure is optimal, but the scheme could lose efficiency already for moderate values of $l$. Therefore, we would like to use the final preconditioner $P_n = P_n^{(l)}$ directly on the original system, with coefficient matrix $A_n$. The following theorem gives a theoretical ground for this choice, showing that $P_n$ is an optimal preconditioner of $A_n$ if, for every $j = 0, \ldots, l-1$, the matrix $P_n^{(j+1)}$ is an optimal preconditioner for $P_n^{(j)}$; this result will be used later on in Theorem 4.1.

**Theorem 3.1.** Let $A_n, P_n$ two positive definite matrices of size $n$. Assume there exist positive definite matrices $P_n^{(0)}, \ldots, P_n^{(l)}$, positive numbers $\alpha_0, \ldots, \alpha_{l-1}$, $\beta_0, \ldots, \beta_{l-1}$, integer numbers $r_0^{-}, \ldots, r_l^{-}, r_0^{+}, \ldots, r_{l-1}^{+}$, $l \geq 1$, such that

- $P_n^{(0)} = A_n$, $P_n^{(l)} = P_n$, $\alpha_j \leq \beta_j$, $j = 1, \ldots, l-1$,
- the eigenvalues $(P_n^{(j+1)})^{-1} P_n^{(j)}$ belong to the interval $[\alpha_j, \beta_j]$ with the exception of $r_j^{-}$ outliers less than $\alpha_j$ and of $r_j^{+}$ outliers larger than $\beta_j$, $j = 0, \ldots, l-1$.

Then, all the eigenvalues of $P_n^{-1} A_n$ belong to the interval $[\alpha, \beta]$, $\alpha = \prod_{j=0}^{l-1} \alpha_j$, $\beta = \prod_{j=0}^{l-1} \beta_j$, with the exception of $r^{-}$ outliers less than $\alpha$ and $r^{+}$ outliers larger that $\beta$,

$$r^{-} = \sum_{j=0}^{l-1} r_j^{-}, \quad r^{+} = \sum_{j=0}^{l-1} r_j^{+}.$$

**Proof.** Let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$$

be the eigenvalues of $P_n^{-1} A_n$ and let $k \in \{r^{+}+1, \ldots, n-r^{-}\}$. Then it suffices to prove that $\lambda_k \in [\alpha, \beta]$. To this end, we make use of min-max and max-min characterization of the eigenvalues of Hermitian matrices and we can use this argument since $P_n^{-1} A_n$ is similar to the Hermitian (indeed positive definite) matrix $P_n^{-1/2} A_n P_n^{-1/2}$. Hence

\begin{equation}
(3.1) \quad \lambda_k = \max_{\dim(V) = k, v \in V, v \neq 0} \min_{v^*} \frac{v^* A_n v}{v^* P_n v},
\end{equation}

\begin{equation}
(3.2) \quad \lambda_k = \min_{\dim(V) = n+1-k, v \in V, v \neq 0} \max_{v^*} \frac{v^* A_n v}{v^* P_n v}.
\end{equation}

Now, for every $j = 0, \ldots, l-1$, set

$$Q_j = (P_n^{(j+1)})^{-1/2} P_n^{(j)} (P_n^{(j+1)})^{-1/2},$$

consider the subspaces $F_j(-)$ spanned by the $r_j^{-}$ eigenvectors of $Q_j$ related to the eigenvalues which are less than $\alpha_j$, and $F_j(+)$ spanned by the $r_j^{+}$ eigenvectors of $Q_j$.
for which the correspondent eigenvalues are greater than $\beta_j$. Then, we define:

$$L(-) = \bigcap_{j=0}^{l-1} \left( P_n^{(j+1)} \right)^{-1/2} [F_j(-)]^\perp,$$

(3.3)

$$L(+) = \bigcap_{j=0}^{l-1} \left( P_n^{(j+1)} \right)^{-1/2} [F_j(+)]^\perp.$$  

(3.4)

By the assumptions, the subspaces $F_j(-)$ and $F_j(+)$ have dimension $r_j^-$ and $r_j^+$, respectively. Thus, $[F_j(-)]^\perp$ and $\left( P_n^{(j+1)} \right)^{-1/2} [F_j(-)]^\perp$ have dimension $n - r_j^+$ while $[F_j(+)]^\perp$ and $\left( P_n^{(j+1)} \right)^{-1/2} [F_j(+)]^\perp$ have dimension $n - r_j^-$. In conclusion, the subspaces $L(-)$ and $L(+)$ defined in (3.3) and (3.4), respectively, have dimensions larger than $n - r_j^-$ and $n - r_j^+$, respectively with $r_j^- = \sum_{j=0}^{l-1} r_j^-$, $r_j^+ = \sum_{j=0}^{l-1} r_j^+$. Since the dimension of such subspaces is large enough, we deduce that $V \cap L(-)$ and $V \cap L(+)$ are non trivial (they have dimension at least equal to 1), with $V$ being any subspace reported in (3.1) and (3.2). Therefore

$$\lambda_k = \max_{\text{dim}(V) = k} \min_{v \in V, v \neq 0} \frac{v^* A_n v}{v^* P_n v} \leq \max_{\text{dim}(V) = k} \min_{v \in V \cap L(+), v \neq 0} \frac{v^* A_n v}{v^* P_n v} = \max_{\text{dim}(V) = k} \min_{v \in V \cap L(+), v \neq 0} \frac{1}{v^* \left( \prod_{j=0}^{l-1} P_n^{(j)} \right) v},$$

$$\leq \prod_{j=0}^{l-1} \beta_j = \beta,$$

$$\lambda_k = \min_{\text{dim}(V) = n+1-k} \max_{v \in V, v \neq 0} \frac{v^* A_n v}{v^* P_n v} \geq \min_{\text{dim}(V) = n+1-k} \max_{v \in V \cap L(-), v \neq 0} \frac{v^* A_n v}{v^* P_n v} = \min_{\text{dim}(V) = n+1-k} \max_{v \in V \cap L(-), v \neq 0} \frac{1}{v^* \left( \prod_{j=0}^{l-1} P_n^{(j)} \right) v},$$

$$\geq \prod_{j=0}^{l-1} \alpha_j = \alpha,$$

and the proof is concluded.

4. The spectrum of $\tau_n^{-1}(f)T_n(f)$. The main theoretical result concerning the ill-conditioned Toeplitz sequences and the proposed $\tau$ preconditioners is stated below.

Theorem 4.1.
Let $f$ be the generating function of $T_n(f)$ having a single zero at zero of order \( \theta \in \mathbb{R}^+ \), and let \( \tau_n(f) \) be the related \( \tau \) matrix as defined in [2,1]. The following facts hold:

1. If \( \theta \in [0,2] \), then there exist constants \( c,C > 0 \) independent of the dimension \( n \), so that \( c \leq \lambda_i(\tau_n^{-1}(f)T_n(f)) \leq C \) for every \( i,n \), i.e., the sequences \( \{\tau_n(f)\}_n \) and \( \{T_n(f)\}_n \) are spectrally equivalent.

2. If \( \theta \in (2,\infty) \) then there exist a constant \( c > 0 \) and a positive number \( m \) such that \( c \leq \lambda_i(\tau_n^{-1}(f)T_n(f)) \) for every \( i,n \). Moreover, at most \( m \) eigenvalues of this preconditioned matrix can grow to infinity. Hence, the essential spectral equivalence between \( \{\tau_n(f)\}_n \) and \( \{T_n(f)\}_n \) holds.

Proof. First, we recall that when \( \theta = 0 \), the generating function is strictly positive and so the spectrum \( \sigma(\tau_n^{-1}(f)T_n(f)) \) is bounded from below and above by constants \( c,C > 0 \) independent of the dimension \( n \), since both matrices are bounded from below and above by constants far away from zero and infinity. The same holds true also when \( \theta = 2 \) since \( f \) is equivalent to \( g_1(t) = 2 - 2 \cos(t) \) in the sense that there exist \( k_1,k_2 > 0 \) for which

\[
k_1g(t) \leq f(t) \leq k_2g(t) \quad \forall t.
\]

Then, it is known from [6] that for the natural \( \tau \) preconditioner, \( \tau_n^{\text{nat}}(f) \), the following inequalities

\[
c_1 < \sigma(\tau_n^{\text{nat}}(g_1))^{-1}T_n(f) < c_2 \quad c_1,c_2 > 0
\]

holds true. So

\[
\hat{c}_1 < \sigma(\tau_n^{-1}(f)T_n(f)) < \hat{c}_2
\]

since

\[
\frac{x^T T_n(f)x}{x^T \tau_n^{\text{nat}}(g_1)x} = \frac{x^T T_n(f)x}{x^T \tau_n(f)x} \frac{x^T \tau_n(f)x}{x^T \tau_n^{\text{nat}}(g_1)x}
\]

and the second term on the right part is bounded far away from zero and infinity, owing to the equivalence of \( g_1 \) and \( f \).

In the case where \( \theta = 4 \), \( f \sim g_2 \) with \( g_2(t) = (2 - 2 \cos(t))^2 \). Following again the above analysis and knowing from [6] that the preconditioned matrix \( [\tau_n^{\text{nat}}(g_2)]^{-1}T_n(f) \) has at most 2 eigenvalues growing to infinity, we conclude that \( \tau_n^{-1}(f)T_n(f) \) will also have at most 2 eigenvalues growing to infinity as \( n \to \infty \). For the convenience of the reader we decouple the complete proof into the following three parts:

a) the maximum eigenvalue of \( \tau_n^{-1}(f)T_n(f) \) is bounded, when \( \theta \in [0,2] \);

b) at most a constant number of eigenvalues of \( \tau_n^{-1}(f)T_n(f) \) can tend to infinity, when \( \theta \in (2,\infty) \);

c) the minimum eigenvalue of \( \tau_n^{-1}(f)T_n(f) \) is bounded from below by a constant independent of \( n \), when \( \theta \) is a real positive number.

Proof of step a) We consider the symmetric positive semidefinite matrix-valued function

\[
F(t) = \begin{pmatrix}
1 & |t| \\
|t| & t^2
\end{pmatrix}
\]

Then, the generated block Toeplitz matrix

\[
B_{2n}(F(t)) = \begin{pmatrix}
T_n(1) & T_n(|t|) \\
T_n(|t|) & T_n(t^2)
\end{pmatrix}
\]
is positive semidefinite and so is its Schur complement

\[ S = T_n(t^2) - T_n(|t|)T_n(|t|) \geq 0 \Rightarrow T_n(t^2) \geq T_n(|t|)T_n(|t|) \]

where the symbol "\geq" stands for the partial ordering in the space of Hermitian matrices (i.e. \(A \geq B\) if and only if \(A - B\) is positive semidefinite). Pre and post multiplying the above inequality with the positive definite \(\tau\) matrix \(\tau_n(|t|^{-1})\), by the inertia law, we get

\[ \tau_n(|t|^{-1})T_n(t^2)\tau_n(|t|^{-1}) \geq \tau_n(|t|^{-1})T_n(|t|)T_n(|t|)\tau_n(|t|^{-1}). \]

The matrix in the left hand side of the inequality above is similar to the preconditioned case of \(\tau_n(t^{-2})T_n(t^2)\). This matrix has bounded spectrum, since it corresponds to the case of \(\theta = 2\). Thus, taking the spectral radii in both sides, we deduce that

\[ C \geq \rho(\tau_n(|t|^{-1})T_n(t^2)\tau_n(|t|^{-1})) \geq \tau_n(|t|^{-1})T_n(|t|)T_n(|t|)\tau_n(|t|^{-1}) \]

\[ = \|\tau_n(|t|^{-1})T_n(|t|)\|_2^2 \geq \rho(\tau_n(|t|^{-1})T_n(|t|))^2. \]

Thus the maximum eigenvalue of \(\tau_n(|t|^{-1})T_n(|t|)\) is bounded from above by the constant \(\sqrt{C}\).

Even though this is a special case and the considered procedure furnishes the upper bound for the concrete case of \(\theta = 1\), the idea can be easily generalized to cover any \(\theta \in (0,2)\).

Let us assume that \(\rho(\tau_n(|t|^{-\theta_1})T_n(|t|^{\theta_1})) \leq C_1\) and \(\rho(\tau_n(|t|^{-\theta_2})T_n(|t|^{\theta_2})) \leq C_2\) for some \(\theta_1, \theta_2 \in [0,2]\). Let also \(\hat{\theta}\) be the arithmetic mean of \(\theta_1, \theta_2\), i.e., \(\hat{\theta} = \frac{\theta_1 + \theta_2}{2}\). Then,

\[ F(t) := \begin{pmatrix} |t|^{\theta_1} & |t|^{\hat{\theta}} \\ |t|^{\hat{\theta}} & |t|^{\theta_2} \end{pmatrix} \geq 0 \Rightarrow B_{2n}(F(t)) := \begin{pmatrix} T_n(|t|^{\theta_1}) & T_n(|t|^{\hat{\theta}}) \\ T_n(|t|^{\hat{\theta}}) & T_n(|t|^{\theta_2}) \end{pmatrix} \geq 0. \]

Hence, the Schur complement of the above block Toeplitz matrix should be positive semidefinite, a fact that is translated into the relation

\[ T_n(|t|^{\theta_2}) \geq T_n(|t|^{\hat{\theta}})T_n^{-1}(|t|^{\theta_1})T_n(|t|^{\hat{\theta}}). \]

Consequently, we pre and post multiply both sides by the positive definite matrix \(\tau_n(|t|^{-\frac{3}{2}})\) and we use the Rayleigh quotients to get

\[ C_2 \geq \frac{y^T \tau_n(|t|^{-\frac{3}{2}})T_n(|t|^{\theta_2})\tau_n(|t|^{-\frac{3}{2}})y}{y^Ty} \geq \frac{y^T \tau_n(|t|^{-\frac{3}{2}})T_n(|t|^{\hat{\theta}})T_n^{-1}(|t|^{\theta_1})T_n(|t|^{\hat{\theta}})\tau_n(|t|^{-\frac{3}{2}})y}{y^Ty}. \]

We multiply and divide the last term in the inequality above by the quantity \(z^Tz\), where \(z = \tau_n(|t|^{-\frac{3}{2}})T_n(|t|^{\hat{\theta}})\tau_n(|t|^{-\frac{3}{2}})y\). Then, this term can be written as

\[ \frac{z^T \tau_n(|t|^{\hat{\theta}})T_n^{-1}(|t|^{\theta_1})\tau_n(|t|^{\hat{\theta}})z}{z^Tz} \geq \frac{1}{\rho(\tau_n(|t|^{-\theta_1})T_n(|t|^{\theta_1}))} \geq \frac{1}{C_1}. \]
We substitute it into inequalities \((4.1)\) and we infer
\[
C_2 C_1 \geq \frac{z^T z}{y^T y} = \frac{y^T \tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}) y}{y^T y}.
\]
(4.2)

This inequality holds also true if we take as \(y\) the eigenvector \(x\) corresponding to the spectral radius \(\rho(\tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}))\). Thus
\[
C_2 C_1 \geq \rho(\tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}))
\]
(4.3)
\[
= \|\tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}})\|_2^2 \geq \rho(\tau_n(|t|^{-\frac{\theta}{2}}) T_n(|t|^\theta) \tau_n(|t|^{-\frac{\theta}{2}}))^2
\]
\[
= \rho(\tau_n(|t|^{-\theta}) T_n(|t|^\theta))^2
\]

and hence we have proven that the spectral radius of the preconditioned matrix \(\tau_n(|t|^{-\theta}) T_n(|t|^\theta)\) has an upper bound the constant \(\sqrt{C_2 C_1}\).

Starting from \(\theta_1 = 0, \theta_2 = 2\), we proved the bound for \(\theta = 1\). Following the very same procedure, we prove the bound for \(\theta = \frac{1}{2}\) and \(\theta = \frac{3}{2}\) and so on. Finally, we can prove the same property for every \(\theta\) rational number in \((0, 2)\) and with the important observation that the bound does not depend on the given rational number: indeed, when dealing with the case \(\theta = 1\), the bound is the geometric mean of the bounds for \(\theta = 0\) and \(\theta = 2\) so that it does not exceed the maximum of the two bounds; by iterating the procedure the same observation is still true. Furthermore, since the set of rational numbers is dense in the set of real numbers, the same property is proven for all \(\theta \in (0, 2)\), because of the continuity of the matrices \(\tau_n(|t|^{-\theta})\) and \(T_n(|t|^\theta)\) with respect to the parameter \(\theta\) and because of the continuity of the spectrum with respect to the matrix coefficients.

**Proof of step b** We use Theorem \(3.1\) with \(l = 4\). More precisely, taking into account that \(\theta > 2\), we write \(\theta = 2k + r, k \geq 1\) integer, \(r \in [0, 2)\), and we define the following \(l\) step preconditioning:

\[
A_n = P_n^{(0)} = T_n(|t|^\theta),
\]
\[
P_n^{(1)} = T_n((2 - 2 \cos(t))^k |t|^r),
\]
\[
P_n^{(2)} = \tau_n((2 - 2 \cos(t))^k T_n(|t|^r),
\]
\[
P_n^{(3)} = \tau_n((2 - 2 \cos(t))^k |t|^r),
\]
\[
P_n^{(4)} = \tau_n(|t|^\theta) = P_n.
\]

Now \(\{P_n^{(1)}\}\) and \(\{A_n = P_n^{(0)}\}\) are spectrally equivalent and the eigenvalues of
\[
\left(P_n^{(1)}\right)^{-1} P_n^{(0)}
\]
belong to the interval \((r, R)\), with
\[
r = \min_{t \in [0, 2\pi]} \frac{|t|^{2k}}{(2 - 2 \cos(t))^k}, \quad R = \max_{t \in [0, 2\pi]} \frac{|t|^{2k}}{(2 - 2 \cos(t))^k}.
\]
(4.4)

\(\{P_n^{(2)}\}\) and \(\{P_n^{(1)}\}\) are essentially spectrally equivalent and indeed their difference has rank bounded by a quantity proportional to \(k\), while the analysis of \(\{P_n^{(3)}\}\) and \(\{P_n^{(2)}\}\) reduces to the one performed in **step b**. Finally \(\{P_n = P_n^{(4)}\}\) and \(\{P_n^{(3)}\}\) are
spectrally equivalent and the eigenvalues of \( \left\{ \left( P_n^{(1)} \right)^{-1} P_n^{(3)} \right\} \) belong to the interval \([1/R, 1/r]\), with \(r, R\) defined in \([4,4]\).

The use of Theorem 3.1 leads to the desired conclusion.

**Proof of step c)** We will prove that \( \lambda_{\min}(\tau^{-1}(|t|^\theta)T(|t|^\theta)) > m \) with constant \( m \) independent of \( n \), by proving that for every normalized vector \( z \in \mathbb{R}^n \), the corresponding Rayleigh quotient \( z^T T_n(|t|^\theta)z \) is bounded from below by \( m \). Using (2.1) and (2.2) and making some simple manipulations, we obtain that the denominator \( D \) of the above ratio can be written as

\[
D = z^T r_n(|t|^\theta)z = (Sz)^T D(Sz) = \frac{2}{n+1} \sum_{k=1}^{n} \left( \frac{k\pi}{n+1} \right)^{\theta} \left( \sum_{j=1}^{n} \sin \left( \frac{jk\pi}{n+1} \right) z_j \right)^2
\]

while the numerator \( N \) can be expanded as

\[
z^T T_n(|t|^\theta)z = \sum_{k=1}^{n} z_k \sum_{j=1}^{n} t_{k-j} z_j = \frac{1}{2\pi} \sum_{k=1}^{n} z_k \sum_{j=1}^{n} \int_{-\pi}^{\pi} |t|^\theta \cos (k-j) t \, dt \, z_j.
\]

Using the trigonometric identity \( \cos (a - b) = \cos a \cos b + \sin a \sin b \), we split the above expression in two positive terms, \( C \) and \( S \), where:

\[
C = \frac{1}{2\pi} \sum_{k=1}^{n} z_k \sum_{j=1}^{n} \left( \int_{-\pi}^{\pi} |t|^\theta \cos (kt) \cos (jt) \, dt \right) z_j = \frac{1}{\pi} \int_{0}^{\pi} |t|^\theta \left( \sum_{j=1}^{n} \cos (jt) z_j \right)^2 \, dt
\]

and the

\[
S = \frac{1}{2\pi} \sum_{k=1}^{n} z_k \sum_{j=1}^{n} \left( \int_{-\pi}^{\pi} |t|^\theta \sin (kt) \sin (jt) \, dt \right) z_j = \frac{1}{\pi} \int_{0}^{\pi} |t|^\theta \left( \sum_{j=1}^{n} \sin (jt) z_j \right)^2 \, dt
\]

Using the trapezoidal rule we can see that the term \( S \) is strongly related to the denominator since

\[
\frac{1}{\pi} \sum_{k=0}^{n} \int_{k\pi/\pi}^{(k+1)\pi/\pi} |t|^\theta \left( \sum_{j=1}^{n} \sin (jt) z_j \right)^2 \, dt \approx \frac{1}{n+1} \sum_{k=1}^{n} \left( \frac{k\pi}{n+1} \right) \left( \sum_{j=1}^{n} \sin \left( \frac{jk\pi}{n+1} \right) z_j \right)^2.
\]

Following an asymptotic analysis analogous to that of Lemma 3.4 in [14], we can bound the minimum eigenvalue by a universal positive constant. \( \square \)

Theorem 4.1 deserves a few remarks. The first observation concerns step b), where the procedure for giving an upper bound to the number of the outliers is indeed an effective algorithm that could be numerically tested. The second remark concerns the non-optimal bound that step b) induces: in fact, as stressed by the numerical experiments, only two outliers show up when \( \theta \in (2,4) \). For filling the gap, we could employ the fine technique in step a): however our initial attempts allowed to give a bound on the number of outlying singular values and this does not lead to the desired result. A possible way for overcoming this difficulty could be the use of the Majorization Theory, concerning the moduli of the eigenvalues and the singular values (see [2] for an elegant and rich treatment of this theory).
5. Numerical Experiments. In this section we report numerical examples that were conducted in order to point out the efficiency of the proposed preconditioners and to confirm the validity of the presented theory. The experiments were carried out using Matlab and in the examples where a linear system is involved the righthand side vector is chosen as \((1 \ 1 \ \cdots \ 1)^T\). Although we have run also our examples with the righthand side being random vectors (and the results are essentially of the same type), we adopt the previous choice in order to present a fair comparison with the methods and numerical tests given in the relevant literature. In all cases, the zero vector was chosen as initial guess for the PCG method and the stopping criterion was the inequality \[ \frac{\|r^{(j)}\|_2}{\|r^{(0)}\|_2} \leq 10^{-7}, \] where \(r^{(j)}\) is the residual vector in the \(j\)th iteration.

In Figure 5.1 we give a snapshot of the asymptotical behavior of the eigenvalues of \(\tau_n^{-1}(f)T_n(f)\) where \(f(t) = |t|^3\) and the matrix \(\tau_n(f)\) is constructed as in (2.1). It is clear, and as the theory predict, that from below the minimum eigenvalue of the sequence \(\{\tau_n^{-1}(f)T_n(f)\}_n\) is bounded by a constant, the main mass of them is clustered around one while at most two of them seem to tend to infinity.

In the next tables, we display the performance of our proposed preconditioner applied to various ill-conditioned Toeplitz systems. In all cases, the coefficient matrix is generated by a function with a unique zero at zero of non-even order \(\theta\). As we have mentioned in the introduction, for these cases there is no suitable optimal PCG method. A non-optimal proposal is presented in [15] where the preconditioner is the band Toeplitz matrix generated by the trigonometric polynomial \((2 - 2\cos(t))^{2k}\) where the number \(k\) is such that the distance \(|2k - \theta|\) is minimum. Following the convergence analysis of the PCG method (see e.g. [1]) and the spectral behavior of the aforementioned preconditioner analyzed extensively in [8], we can easily conclude that in our case it is better to overestimate \(\theta\) rather than to underestimate it. The reason is that in the latter case \(O(n)\) eigenvalues of the preconditioned matrix will tend to infinity, while in the first case \(O(n)\) eigenvalues will tend to zero. We denote the preconditioner proposed in [15] as \(S\) while our preconditioner is shortly indicated with the symbol \(\tau\). For our experiments we have chosen the following generating functions:

\[
 f_1(t) = |t|, \quad f_2(t) = |t|^2, \quad f_3(t) = |t|^3, \quad f_4(t) = |t|^\frac{9}{2}.
\]
The corresponding iterations are reported on Tables 5.1, 5.2, 5.3, 5.4. For all the examples, we remark that the unpreconditioned CG method requires a number of iterations exceeding 1000, even for moderate matrix-sizes like \( n = 512 \).

**Table 5.1**
Number of iterations for \( f(t) = |t| \), the extreme eigenvalues of \( P_n^{-1}(f)T_n(f) \) and the number of unbounded eigenvalues.

| n     | S  | \( \tau \) | \( \lambda_{\min} \) | \( \lambda_{\max} \) | \( \sharp \{ \lambda_i(P) \} > 2 \) |
|-------|----|------------|----------------|----------------|-----------------|
| 256   | 33 | 6          | 0.61           | 1.04           | 0               |
| 512   | 44 | 6          | 0.60           | 1.04           | 0               |
| 1024  | 63 | 6          | 0.59           | 1.04           | 0               |
| 2048  | 89 | 6          | 0.59           | 1.04           | 0               |
| 4096  | 124| 7          | 0.58           | 1.04           | 0               |

**Table 5.2**
Number of iterations for \( f(t) = |t|^3 \), the extreme eigenvalues of \( P_n^{-1}(f)T_n(f) \) and the number of unbounded eigenvalues.

| n     | S  | \( \tau \) | \( \lambda_{\min} \) | \( \lambda_{\max} \) | \( \sharp \{ \lambda_i(P) \} > 2 \) |
|-------|----|------------|----------------|----------------|-----------------|
| 256   | 9  | 34         | 1              | 6.4            | 2               |
| 512   | 9  | 51         | 1              | 7.4            | 2               |
| 1024  | 9  | 78         | 1              | 8.5            | 2               |
| 2048  | 10 | 118        | 1              | 9.8            | 2               |
| 4096  | 10 | 179        | 1              | 11.2           | 2               |

**Table 5.3**
Number of iterations for \( f(t) = |t|^7 \), the extreme eigenvalues of \( P_n^{-1}(f)T_n(f) \) and the number of unbounded eigenvalues.

| n     | S  | \( \tau \) | \( \lambda_{\min} \) | \( \lambda_{\max} \) | \( \sharp \{ \lambda_i(P) \} > 2 \) |
|-------|----|------------|----------------|----------------|-----------------|
| 256   | 20 | 9          | 1              | 32.2           | 2               |
| 512   | 24 | 10         | 1              | 46.5           | 2               |
| 1024  | 31 | 10         | 1              | 66.9           | 2               |
| 2048  | 40 | 11         | 1              | 96.3           | 2               |
| 4096  | 52 | 11         | 1              | 137.8          | 2               |

**Table 5.4**
Number of iterations for \( f(t) = |t|^{9/2} \), the extreme eigenvalues of \( P_n^{-1}(f)T_n(f) \) and the number of unbounded eigenvalues.

| n     | S  | \( \tau \) | \( \lambda_{\min} \) | \( \lambda_{\max} \) | \( \sharp \{ \lambda_i(P) \} > 2 \) |
|-------|----|------------|----------------|----------------|-----------------|
| 256   | 45 | 10         | 0.77           | 1.1 \times 10^3 | 2               |
| 512   | 62 | 11         | 0.74           | 3.0 \times 10^3 | 2               |
| 1024  | 86 | 13         | 0.72           | 8.5 \times 10^3 | 2               |
| 2048  | 119| 14         | 0.70           | 2.4 \times 10^4 | 2               |
| 4096  | 165| 14         | 0.69           | 6.8 \times 10^4 | 2               |

An important point is that in all considered cases, we only observed 2 outliers, showing that there is room for theoretical improvement in Theorem 4.1.
6. Concluding remarks. In previous works, the spectral equivalence of the matrix sequences \( \{\tau_n(f)\}_n \) and \( \{T_n(f)\}_n \) was proven under the assumption that the symbol \( f \) has a zero of order 2 at zero: furthermore, if the order \( \theta \) is an even number larger than 2, the essential spectral equivalence was proved. Here we have expanded the previous result to any positive order \( \theta \), by showing that the spectral equivalence holds for \( \theta \leq 2 \) and the essential spectral equivalence can be proven for every \( \theta > 2 \).

A possible line of further research could concern extending the validity of the proposed idea also to other trigonometric matrix algebras, (e.g., the circulant algebra) and the multi-level case. Obviously, more difficulties are expected on this directions due to the facts that the \( \tau \) algebra is closer in a rank sense to the Toeplitz structure, when the generating function of the latter is a even trigonometric polynomial, and, due to the negative results that hold in the multidimensional case (see [19], [13]). Furthermore, concerning Theorem 4.1, the proof technique used in step a) is rather precise for \( \theta \in [0, 2] \), but it did not work for larger values of \( \theta \); a further investigation in this direction would be useful in order to prove a precise bound on the number of outliers, since Theorem 3.1 used in step b) provides a non-optimal estimate, as suggested by the numerical tests.

REFERENCES

[1] O. Axelsson and G. Lindskog, On the rate of convergence of the preconditioned conjugate gradient method, Numer. Math., 48 (1986), pp. 499–523.
[2] R. Bhatia, Matrix Analysis, Springer-Verlag, New York, 1997.
[3] D. A. Bini and M. Capovani, Spectral and computational properties of band symmetric Toeplitz matrices, Linear Algebra Appl., 52 (1983), pp. 99–126.
[4] D. A. Bini and F. Di Benedetto, A new preconditioner for the parallel solution of positive definite Toeplitz systems, Proc. 2nd SPAA, ACM Press., (1990), pp. 120–123. Crete, Greece.
[5] R. H. Chan and X.-Q. Jin, An Introduction to Iterative Toeplitz Solvers, Society for Industrial and Applied Mathematics, Philadelphia, PA, 2007.
[6] F. Di Benedetto, Analysis of preconditioning techniques for ill-conditioned Toeplitz matrices, SIAM J. Sci. Comput., 16 (1995), pp. 682–697.
[7] F. Di Benedetto, G. Fiorentino, and S. Serra Capizzano, C.G. preconditioning of Toeplitz matrices, Comput. Math. Appl., 25 (1993), pp. 35–45.
[8] F. Di Benedetto and S. Serra Capizzano, A unifying approach to abstract matrix algebra preconditioning, Numer. Math, 82 (1999), pp. 57–90.
[9] M. Donatelli, C. Garoni, C. Manni, S. Serra-Capizzano, and S. H., Robust and optimal multi-iterative techniques for IgA Galerkin linear systems, Computer Methods in Applied Mechanics and Engineering.
[10] T. Huckle, Iterative methods for ill-conditioned Toeplitz matrices, Calcolo, 33 (1996), pp. 177–190.
[11] M. Miranda and P. Tilli, Asymptotic spectra of hermitian block Toeplitz matrices and preconditioning results, SIAM J. Matrix Anal. Appl., 21 (2000), pp. 867–881.
[12] M. K. Ng, Iterative Methods for Toeplitz Systems (Numerical Mathematics and Scientific Computation), Oxford University Press, Inc., New York, NY, USA, 2004.
[13] D. Noutsos, S. Serra Capizzano, and P. Vassalos, Matrix algebra preconditioners for multilevel Toeplitz systems do not insure optimal convergence rate., Theoret. Computer Sci., 315 (2004), pp. 557–579.
[14] D. Noutsos and P. Vassalos, Superlinear convergence for PCG using band plus algebra preconditioners for Toeplitz systems, Computers and Mathematics with Applications, 56 (2008), pp. 1255–1270.
[15] S. Serra Capizzano, New PCG based algorithms for the solution of hermitian Toeplitz systems, Calcolo, 32 (1995), pp. 153–176.
[16] — , New PCG based algorithms for the solution of Hermitian Toeplitz systems, Calcolo, 32 (1995), pp. 154–176.
[17] — , Spectral and computational analysis of block Toeplitz matrices having nonnegative definite matrix-valued generating functions., BIT, 39 (1999), pp. 152–175.
[18] ——, *Superlinear PCG methods for symmetric Toeplitz systems*, Math. Comp., 68 (1999), pp. 793–803.

[19] S. Serra Capizzano and E. Tyrtyshnikov, *Any circulant-like preconditioner for multilevel matrices is not superlinear*, SIAM J. Matrix Anal. Appl., 21 (1999), pp. 431–439.