Essential spectral equivalence via multiple step preconditioning and applications to ill conditioned Toeplitz matrices

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The scope of this work

The main objective 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 $\theta \in \mathbb{R}$: the entry $(j, k)$, $1 \leq j, k \leq n$, of the matrix $T_n(f)$ is the $s$-th Fourier coefficient of $f$ with $s = j - k$ and

$$a_s = \frac{1}{2\pi} \int_0^{2\pi} f(t)e^{-ist} \, dt.$$

We focusing on the preconditioners belonging to $\tau$ algebra (the set of all real symmetric matrices diagonalized by the sine transform), we study the spectrum of the matrix sequences

$$\{A_n\}_n$$

with $A_n = \tau^{-1}_n(f)T_n(f)$ with the goal being the localizing of its eigenvalues and understanding their asymptotic behavior.
Importance

We recall that the theoretical analysis of such a matrix sequence gives precise information on the convergence speed of the related preconditioned Conjugate Gradient (PCG) method. In addition the associated preconditioning strategy can be used in connection with multigrid schemes. Concrete example of the latter is the use of fast Toeplitz preconditioning in the context of a multigrid method for a Galerkin isogeometric analysis approximation to the solution 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.
In the literature, there are dozens of papers that extensively analyze the problem of understanding the spectrum of \( \{A_n\}_n \), under the assumption that 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. This is the novel contribution of this work.
Preliminaries definitions

The preconditioners that we are focus on belong to $\tau$ algebra. Specifically the sequence $\{P_n\}_n$ is constructed as

$$P_n = \tau_n(f) = S_n \text{diag}(f(w^{[n]})) S_n$$  \hfill (1)

where $w^{[n]}$ 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

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

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 $w^{[n]}$. 
Preliminaries definitions

Definition

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 \(\beta\).
Two cases

We study the spectral properties of the preconditioned matrix sequence \( \{A_n\}_n = \{\tau_n^{-1}(f) T_n(f)\}_n \), by dividing the analysis into two steps:

a) we consider the case where the order of the zero is \( \theta \in (0, 2] \) and then,

b) using a multiple step preconditioning, we consider the case \( \theta > 2 \), which is somehow reduced to the first case.

As a result, we 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 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 concerning the idea of the multiple step preconditioning
Results from Block Toeplitz matrices

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. Even though the resulting structure, and consequently its spectral properties, are quite different from the ones of the scalar and multi-level Toeplitz forms, there is a strong link with the one-level Toeplitz matrices generated by a matrix-valued function, since 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 $T_n(F)$. 
Results from Block Toeplitz matrices

Furthermore, 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. This property is used in connection with Schur complement mainly to show that when $\theta \in [0, 2]$ the maximum eigenvalue of $\tau_n^{-1}(f) T_n(f)$ is bounded by a constant for every $n$. 
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), $j = 0, \ldots, l - 1, P_n^{(0)} = A_n$.

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 $A_n$. 
We use the previous theorem with $l = 4$ in the case where $\theta > 2$. Then, we can write $\theta = 2k + r$, $k \geq 1$ integer, $r \in [0, 2)$, and we define the following $l$ step preconditioning:

\[
\begin{align*}
A_n &= P_n^{(0)} = T_n(|t|^\theta), \\
P_n^{(1)} &= T_n((2 - 2 \cos(t))^k |t|^r), \\
P_n^{(2)} &= \tau_n((2 - 2 \cos(t))^k) T_n(|t|^r), \\
P_n^{(3)} &= \tau_n((2 - 2 \cos(t))^k |t|^r), \\
P_n^{(4)} &= \tau_n(|t|^\theta) = P_n.
\end{align*}
\]
The following theorem gives a theoretical ground for this choice, showing that $P_n$ is an optimal preconditioner of $A_n$.

**Theorem**

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

- $P_n^{(0)} = A_n, P_n^{(l)} = P_n, \alpha_j \leq \beta_j, j = 1, \ldots, l - 1$,
- the eigenvalues $\left(P_n^{(j+1)}\right)^{-1} P_n^{(j)}$ 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,

$$
\sigma(P_n^{-1}A_n) \in [\alpha, \beta], \quad \alpha = \prod_{j=0}^{l-1} \alpha_j, \quad \beta = \prod_{j=0}^{l-1} \beta_j
$$

, with the exception of $r^{-}$ outliers less than $\alpha$ and $r^{+}$ outliers larger that $\beta$.
The spectrum of \( \{\tau_n^{-1}(f) T_n(f)\}_n \)

**Theorem**

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 (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.
Sketch of proof

The main proof can be decoupled 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.
Numerical Experiments

The experiments were carried out using Matlab and in the examples where a linear system is involved the righthand side vector is chosen as \((1\ 1\ \cdots\ 1)^T\). 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 the next figure 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 we proposed.
Figure: Spectrum of $\tau_n(f)^{-1} T_n(f)$, where $f(t) = |t|^3$
First Example

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

<table>
<thead>
<tr>
<th>n</th>
<th>S</th>
<th>$\mathcal{T}$</th>
<th>$\lambda_{\min}$</th>
<th>$\lambda_{\max}$</th>
<th>$#{\lambda_i(P)} &gt; 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>256</td>
<td>33</td>
<td>6</td>
<td>0.61</td>
<td>1.04</td>
<td>0</td>
</tr>
<tr>
<td>512</td>
<td>44</td>
<td>6</td>
<td>0.60</td>
<td>1.04</td>
<td>0</td>
</tr>
<tr>
<td>1024</td>
<td>63</td>
<td>6</td>
<td>0.59</td>
<td>1.04</td>
<td>0</td>
</tr>
<tr>
<td>2048</td>
<td>89</td>
<td>6</td>
<td>0.59</td>
<td>1.04</td>
<td>0</td>
</tr>
<tr>
<td>4096</td>
<td>124</td>
<td>7</td>
<td>0.58</td>
<td>1.04</td>
<td>0</td>
</tr>
</tbody>
</table>

S : The best non-optimal preconditioner in the literature (proposed by S. Serra Capizzano) generated by the trigonometric polynomial $(2 - 2 \cos(t))^{2k}$ where the number $k$ is such that the distance $|2k - \theta|$ is minimum.

$\mathcal{T}$ : Our $\tau$ preconditioner.
Second example

**Table:** Number of iterations for $f(t) = |t|^{\frac{7}{2}}$, the extreme eigenvalues of $P_{n}^{-1}(f)T_{n}(f)$ and the number of unbounded eigenvalues.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$S$</th>
<th>$\tau$</th>
<th>$\lambda_{\text{min}}$</th>
<th>$\lambda_{\text{max}}$</th>
<th>$#{\lambda_i(P)} &gt; 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>256</td>
<td>20</td>
<td>9</td>
<td>1</td>
<td>32.2</td>
<td>2</td>
</tr>
<tr>
<td>512</td>
<td>24</td>
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<tr>
<td>1024</td>
<td>31</td>
<td>10</td>
<td>1</td>
<td>66.9</td>
<td>2</td>
</tr>
<tr>
<td>2048</td>
<td>40</td>
<td>11</td>
<td>1</td>
<td>96.3</td>
<td>2</td>
</tr>
<tr>
<td>4096</td>
<td>52</td>
<td>11</td>
<td>1</td>
<td>137.8</td>
<td>2</td>
</tr>
</tbody>
</table>
Third example

Table: 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.

<table>
<thead>
<tr>
<th>n</th>
<th>S</th>
<th>( \tau )</th>
<th>( \lambda_{\text{min}} )</th>
<th>( \lambda_{\text{max}} )</th>
<th>#{\lambda_i(P)} &gt; 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>256</td>
<td>45</td>
<td>10</td>
<td>0.77</td>
<td>(1.1 \times 10^3)</td>
<td>2</td>
</tr>
<tr>
<td>512</td>
<td>62</td>
<td>11</td>
<td>0.74</td>
<td>(3.0 \times 10^3)</td>
<td>2</td>
</tr>
<tr>
<td>1024</td>
<td>86</td>
<td>13</td>
<td>0.72</td>
<td>(8.5 \times 10^3)</td>
<td>2</td>
</tr>
<tr>
<td>2048</td>
<td>119</td>
<td>14</td>
<td>0.70</td>
<td>(2.4 \times 10^4)</td>
<td>2</td>
</tr>
<tr>
<td>4096</td>
<td>165</td>
<td>14</td>
<td>0.69</td>
<td>(6.8 \times 10^4)</td>
<td>2</td>
</tr>
</tbody>
</table>
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 D.Noutsos&S.Serra Capizzano&P.Vassalos, 2004,TCS).
Thank you very much for your attention!