PRECONDITIONING BLOCK TOEPLITZ MATRICES[*]

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Abstract. We investigate the spectral behavior of preconditioned block Toeplitz matrices with small non-Toeplitz blocks. These matrices have a quite different behavior than scalar or mulitlevel Toeplitz matrices. Based on the connection between Toeplitz and Hankel matrices we derive some negative results on eigenvalue clustering for ill-conditioned block Toeplitz matrices. Furthermore, we identify Block Toeplitz matrices that are easy to solve by the preconditioned conjugate gradient method. We derive some useful inequalities that give information on the location of the spectrum of the preconditioned systems. The described analysis also gives information on preconditioning ill-conditioned Toeplitz Schur complement matrices and Toeplitz normal equations.

Key words. Toeplitz, block Toeplitz, Schur complement, preconditioning, conjugate gradient method

AMS subject classifications. 65F10, 65F15

1. Introduction. We consider ill-conditioned symmetric positive definite (spd) block Toeplitz (BT) matrices of the form

$$
(1.1) \qquad B_n = \begin{pmatrix} A_0 & A_{-1} & \cdots & \cdots & A_{1-n} \\ A_1 & A_0 & A_{-1} & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & A_{-1} \\ A_{n-1} & \cdots & \cdots & A_1 & A_0 \end{pmatrix}
$$

with small general $k \times k$ matrices A_j, $j = 1 - n, \ldots, n - 1$, k fixed and independent of n. Mainly, we are interested in the case $k = 2$, because for this case we can display already all the problems and techniques that are different from the scalar case with $k = 1$.

Furthermore, we assume that the family of BT matrices $B_n = B_n(F)$, $n = 1, 2, 3, \ldots$, is related to a generating $k \times k$ matrix function

$$
F(x) = (f_{j,m}(x))_{j,m=1}^k = \cdots + A_1 \exp(-ix) + A_0 + A_{-1} \exp(ix) + \cdots
$$

that may be L^1, L^2, L^∞, or continuous and 2π periodic in the interval $[-\pi, \pi]$, which is equivalent to write that every $f_{j,m}(x)$, $j, k = 1, \ldots, k$, is L^1, L^2, L^∞, or continuous and 2π-periodic in $[-\pi, \pi]$ as standard scalar-valued functions.

By a simple permutation we can transform the matrix B_n into the $k \times k$ block form

$$
(1.2) \qquad \tilde{B}_n = \begin{pmatrix} T_{1,1} & \cdots & T_{1,k} \\ \vdots & & \vdots \\ T_{k,1} & \cdots & T_{k,k} \end{pmatrix}
$$

with $n \times n$ Toeplitz matrices $T_{j,m} = T_{j,m}^{(n)}$, $j, m = 1, \ldots, k$, related to the same generating matrix function $F(x)$. Then, each $f_{j,m}(x)$ is the scalar generating function to $T_{j,m}^{(n)}$.

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Note, that in contrast to multilevel Toeplitz matrices we consider in (1.1) blocks A_j of fixed size that will be in general of non-Toeplitz structure. Hence, the analysis derived for the multilevel case based on trigonometric polynomials [8, 9, 15] cannot be applied in this BT case. In fact such negative results as in [8, 9, 15] do not hold in the block case; see [10, 12] for related positive results concerning strong clustering with block circulant preconditioners and spectral equivalence with band block Toeplitz preconditioners, respectively. So, the BT case is quite different from the scalar case and the multilevel case.

Block Toeplitz matrices are closely related to Schur complements in Toeplitz matrices, e.g., Toeplitz Schur complement $T_1 - T_2 * T_4^{-1} * T_3$ to BT matrix $\begin{pmatrix} T_1 & T_2 \\ T_3 & T_4 \end{pmatrix}$. So, for $k = 2$ the given block equations can be reduced to solving Toeplitz matrices and Schur complement systems of Toeplitz matrices. In the following we will derive theoretical and numerical results on block Toeplitz systems and also on Toeplitz Schur complements. Note, that also the Toeplitz normal equations are a special case of a Schur complement, and therefore are related to block Toeplitz systems.

For a well-conditioned spd Toeplitz matrix T_n related to a continuous generating function $f(x)$ there exist various preconditioning techniques that ensure fast convergence of the preconditioned conjugate gradient (pcg) method; see [2, 7] and the references therein. Fast Transform preconditioners based on circulant matrices or other classes of matrix algebras lead to a preconditioned system with clustered eigenvalues for $C_n^{-1}T_n$. Here the computation of the preconditioner and each step in the pcg algorithm take $O(n \log(n))$ operations based on fast algorithms for the trigonometric transforms. Hence, if the linear system can be solved in a bounded number of iterations - independent of n - then the whole procedure takes $O(n \log(n))$ operations [2, 7]. This case occurs if the symbol is strictly positive or if it is nonnegative and polynomial.

Another important class of preconditioners for ill-conditioned matrices is based on banded Toeplitz matrices. If the scalar generating function $f(x)$ has only zeros of even order then we can define a trigonometric polynomial p that has the same zeros of the same order as f. Then, p is related to a band Toeplitz matrix. Furthermore, the preconditioned system $P_n^{-1}T_n$ is well-conditioned with eigenvalues contained in an interval given by the range of $f(x)/p(x)$; this again leads to fast convergence of the pcg method [3, 10]. In [12] the author considers also band preconditioners with bandwidth up to $\log(n)$ by choosing, e.g., the partial Fourier polynomial $F_n(x)$ for the given Fourier expansion of $F(x)$. For well-conditioned matrices this approach leads to clustered spectrum of the preconditioned system. For ill-conditioned matrices with singular $F(x)$ the banded approximation given by $F_n(x)$ may be indefinite and therefore in [11, 12] a generalization of the approach in [10] is considered in order to deal with the ill-conditioned case; see Theorems 3.1, 3.6, and sections 4.1, 4.2 in [11] and sections 3 and 4 in [12]. Here, we introduce a different banded approximation that can deal with singular $F(x)$ also allowing a broader bandwidth.

Aim of this paper is to generalize the positive preconditioning results for circulant and band preconditioners for Block Toeplitz matrices, e.g., [6, 11, 12, 13, 14], and to derive further results on the eigenvalue distribution and clustering of preconditioned block Toeplitz systems and Toeplitz Schur complements (like the normal equations). This also leads to some negative results on the eigenvalue clustering of preconditioned BT matrices. The paper is organized as follows. In section 2 some results are presented concerning BT, Hankel Matrices and Schur complements of BT matrices. In section 3 some spectral and convergence properties are presented and proved for pcg method applied on BT systems and for preconditioning Toeplitz Schur complements. General propositions for constructing efficient prconditioners for BT systems and Schur complements are given in section 4. In section 5 numerical examples

are presented showing the validity of the theory. Finally, concluding remarks are given in
section 6.

2. Toeplitz, Block Toeplitz and multilevel Toeplitz matrices.
In this section we present
some useful known results that are necessary to obtain the main results in the following sections.

THEOREM 2.1 (Spectrum of preconditioned BT system, Theorem 4.1 in [6], see also [11,
12]). *Let $T_n(G)$ and $T_n(F)$ be two sequences of matrices generated by Lebesgue integrable
Hermitian $k \times k$-matrix-valued functions F and G defined on $Q = [-\pi, \pi]$, where G is
positive definite for almost every $x \in Q$, that is, the Lebesgue measure of $Q \backslash Q_+$ is zero with
$Q_+ := \{x \in Q : G(x) \ spd\}$. Then all the eigenvalues of $T_n^{-1}(G)T_n(F)$ lie in the (not
necessarily bounded) interval $[r, R]$, where*

$$r = \sup\{y \in \mathbf{R} : \lambda_{\mathbf{min}}(\mathbf{G^{-1}F}) > \mathbf{y} \text{ for almost every } \mathrm{x} \in \mathrm{Q_+}\}$$
$$R = \inf\{y \in \mathbf{R} : \lambda_{\mathbf{max}}(\mathbf{G^{-1}F}) < \mathbf{y} \text{ for almost every } \mathrm{x} \in \mathrm{Q_+}\}$$

THEOREM 2.2 (Product of Toeplitz matrices [19]). *If $f, g \in L^\infty$, then*

$$T_n(fg) - T_n(f) * T_n(g) = P_n * H(f) * H(\bar{g}) * P_n + Q_n * H(\bar{f}) * H(g) * Q_n$$

*with $P_n(x_1, \ldots) = (x_1, \ldots, x_n)$ and $Q_n(x_1, \ldots) = (x_n, \ldots, x_1)$ are matrices picking out
the first n entries of an infinite vector, and the infinite Hankel matrix*

$$H(f) = \begin{pmatrix} t_1 & t_2 & t_3 & \cdot \\ t_2 & t_3 & \cdot & \\ t_3 & \cdot & & \\ \cdot & & & \end{pmatrix} .$$

COROLLARY 2.3 (Product of band Toeplitz and Toeplitz matrix). *For a real trigonomet-
ric polynomial $p(x)$ and $g \in L^\infty$ it holds*

$$T_n(pg) = T_n(p)T_n(g) + R_1$$

and

$$T_n^{-1}(p)T_n(pg) = T_n(g) + R_2$$

*with R_j, $j = 1, 2$, matrices of low rank that depends only on $p(x)$ and not on the dimension
n.*

COROLLARY 2.4 (Product of band BT matrix and BT matrix). *For a real trigonometric
matrix polynomial $P(x)$ and $G \in L^\infty$ with $k \times k$ blocks it holds*

$$T_n(PG) = T_n(P)T_n(G) + R_1$$

and

$$T_n^{-1}(P)T_n(PG) = T_n(G) + R_2$$

with R_j, $j = 1, 2$, matrices of low rank.

THEOREM 2.5 (Spectrum of Hilbert matrix [18, 7]). *Let H_n be the $n \times n$ Hilbert matrix
to $H(f)$ with $t_j = 1/j$, $j = 1, 2, \ldots$. Then for any $0 < \epsilon < \pi$, the number of eigenvalues of
H_n with absolute values exceeding ϵ is given by*

$$\frac{2}{\pi} \log n * \operatorname{sech}^{-1} \frac{\epsilon}{\pi} * (1 + o(n)) .$$

Hence for every cluster of eigenvalues around zero with small radius ϵ the number of outliers is growing like $\log(n)$. This behavior is denoted as weakly clustered because the number of outliers is allowed to grow like $o(n)$.

THEOREM 2.6 (Negative results for multilevel Toeplitz matrices [8, 9, 15]). *For ill-conditioned positive definite multilevel Toeplitz matrices there exist examples where for every positive definite multilevel circulant preconditioner there holds:*

1. If the spectrum of the preconditioned matrix is bounded ($\lambda_{\max} \leq \alpha < \infty$, α independent of n), then $\lambda_{min} \to 0$ and $\alpha(n)$ eigenvalues tend to zero, with $\alpha(n)$ tending to infinity when n tends to infinity.

2. If the spectrum of the preconditioned matrix is bounded from below ($\lambda_{\min} \geq \beta > 0$, β independent of n), then $\lambda_{max} \to \infty$ and $\beta(n)$ eigenvalues tend to infinity, with $\beta(n) \to \infty$ for $n \to \infty$.

Now, let us turn to Schur complements related to BT matrices for $k = 2$. The close relationship between BT matrices and Schur complements is displayed by the equations

$$\begin{pmatrix} T_1 & T_2 \\ T_2^H & T_3 \end{pmatrix} = \begin{pmatrix} I & T_2 T_3^{-1} \\ 0 & I \end{pmatrix} * \begin{pmatrix} S_1 & 0 \\ 0 & T_3 \end{pmatrix} * \begin{pmatrix} I & 0 \\ T_3^{-1} T_2^H & I \end{pmatrix} =$$

$$= \begin{pmatrix} I & 0 \\ T_2^H T_1^{-1} & I \end{pmatrix} * \begin{pmatrix} T_1 & 0 \\ 0 & S_3 \end{pmatrix} * \begin{pmatrix} I & T_1^{-1} T_2 \\ 0 & I \end{pmatrix} =$$

$$(2.1) \qquad = \begin{pmatrix} S_1 & 0 \\ 0 & S_3 \end{pmatrix} * \begin{pmatrix} T_1 & -T_2 \\ -T_2^H & T_3 \end{pmatrix}^{-1} * \begin{pmatrix} T_1 & 0 \\ 0 & T_3 \end{pmatrix}$$

with $S_1 = T_1 - T_2 T_3^{-1} T_2^H$ and $S_3 = T_3 - T_2^H T_1^{-1} T_2$. Hence, an efficient preconditioner for a BT matrix directly leads to an efficient preconditioner for both Schur complements S_1 and S_3. On the other side an efficient preconditioner for one of the Schur complements directly leads to an efficient preconditioner for the whole BT matrix.

3. BT matrices and Toeplitz Schur Complements. First we present some useful results on the location of eigenvalues of Schur complements of Toeplitz matrices. These results are based on the connection between Schur complements and block matrices.

THEOREM 3.1 (Preconditioned normal equations). *Consider the family of Toeplitz matrices $T_n(f)$, $n = 1, 2, \ldots$ with generating function f, real Lebesgue integrable. Then it holds*

$$T_n(f^2) \geq T_n(f)^2 .$$

Proof. We consider the BT matrix B_n to

$$F(x) := \begin{pmatrix} 1 & f(x) \\ f(x) & f^2(x) \end{pmatrix} .$$

This matrix F is rank-1 symmetric positive semidefinite with eigenvalues $\lambda = 0$ and $\lambda = 1 + f(x)^2$. The generating function is positive semidefinite, therefore the BT matrix B_n is also positive semidefinite. Hence, both Schur complements are positive semidefinite and therefore $T_n(f^2) - T_n^2(f) \geq 0$ and $I_n - T_n(f) T_n^{-1}(f^2) T_n(f) \geq 0$ (for $T_n(f^2)$ nonsingular). □

Note that if $F(x) \geq 0$ is symmetric positive semidefinite, $B_n(F)$ may be even positive definite, depending on f, e.g., $f(x) = x^2$. Theorem 3.1 can be also shown for general Toeplitz matrices: $T_n(|f|^2) \geq T_n^H(f) T_n(f)$.

LEMMA 3.2. *Consider b, g Lebesgue integrable and $g(x)$ nonnegative with $|b(x)|^2/g(x) < \infty$ for all x, and $T_n(g)$ and $T_n(|b|^2/g)$ nonsingular. Then it holds*

$$T_n(|b|^2/g) \geq T_n^H(b) T_n^{-1}(g) T_n(b)$$

and

$$T_n(g) \geq T_n(b)T_n^{-1}(|b|^2/g)T_n^H(b) \ .$$

Proof. Consider the BT matrix B_n to

$$F(x) = \begin{pmatrix} |b(x)|^2/g(x) & \bar{b}(x) \\ b(x) & g(x) \end{pmatrix} \ . \qquad \square$$

THEOREM 3.3 (Preconditioned Toeplitz Schur Complement). *Let f, g, b Lebesgue integrable and g nonnegative, $|b|^2/g < \infty$, and the matrices $T_n(g)$, $T_n(|b|^2/g)$, $T_n(f - |b|^2/g)$ all nonsingular. Then it holds for the Toeplitz Schur complement relative to the matrix $F(x) := \begin{pmatrix} f & \bar{b} \\ b & g \end{pmatrix}$:*

$$T_n(f - \frac{|b|^2}{g}) \leq T_n(f) - T_n^H(b)T_n^{-1}(g)T_n(b) =: S_n(f,g,b) \ .$$

The eigenvalues of the Toeplitz preconditioned Toeplitz Schur complement

$$T_n(f - |b|^2/g)^{-1} S_n(f,g,b)$$

are greater or equal 1.

Proof. Direct Corollary of Lemma 3.2. $\square$

Note, that for Toeplitz matrices with generating function $f(x)$ equals zero on a whole interval, all matrices $T_n(f)$ will be singular. Furthermore, if in the scalar case $f(x)$ has only isolated zeros of polynomial order then the smallest eigenvalue tends to zero polynomially depending on the order of the zeros of f. The next theorem displays a basic difference between scalar Toeplitz matrices and BT matrices. To prove this Theorem we need the following Lemma

LEMMA 3.4. *If f is a 2π periodic continuous function, then the eigenvalues of $T_n(f^2) - T_n(f)^2$ are clustered at zero and the minimal eigenvalue tends to zero exponentially.*

Proof. The related Hankel matrix is a compact operator; see [1]. Therefore, the sum of the eigenvalues of the Hankel matrix is bounded which guarantees the strong clustering, e.g., the infinite Hilbert matrix is a bounded operator [4, 17, 18]. Furthermore, Tyrtyshnikov has shown in [17] that the smallest eigenvalue of the associated Hankel matrix $H(f)$ tends to zero exponentially. $\square$

THEOREM 3.5 (Ill-posed BT matrix). *There exist examples with generating function $F(x) \geq 0$ but $\det(F(x)) = 0$ such that the related BT matrices $B_n(F)$ are spd. For such a B_n the condition number may grow exponentially with n, resp. the smallest eigenvalue may tend to zero exponentially.*

Proof. As example we consider $B_n(F)$ to generating function $F = \begin{pmatrix} 1 & f \\ f & f^2 \end{pmatrix}$. Then the smallest eigenvalue of B_n can be bounded from above by the smallest eigenvalue of the Schur complement $T_n(f^2) - T_n(f)^2 \geq 0$ which is exponetially converging to zero following the previous Lemma 3.4. (To see the relationship between the spectrum of a natrix and the spectrum of the Schur complement we can consider the Rayleigh quotient). As special example we can choose $f(x) = x^2$. Then $F(x)$ is singular for all x, but $B_n(F)$ is still spd in view of Theorem 2.2. $\square$

Now we want to analyse the spectrum of different preconditioned BT matrices. The first results show, that well-conditioned BT matrices behave similar to scalar Toeplitz matrices.

THEOREM 3.6 (Well-conditioned BT, Theorems 8.4 and 9.3 in [13]). *For well-conditioned spd BT with $F(x)$ 2π-periodic continuous the optimal block circulant preconditioner leads to a strongly clustered spectrum.*

THEOREM 3.7. *Let $f \geq 0$ be real 2π-periodic continuous with a finite number of zeros of even order and $T_n(f^2)$ nonsingular. Then the spectrum of $B_n = T_n(f)T_n^{-1}(f^2)T_n(f)$ is strongly clustered around* 1.

Proof. We can write $f(x) = p(x)h(x)$ with $h(x) \geq m > 0$ and trigonometric polynomial $p(x)$. Then $T_n(f) = T_n(ph) = T_n(p) * T_n(h) + R_1 = T_n(h) * T_n(p) + R_2$ with R_j of low rank (Lemma 2.3). In the same way, $T_n(f^2)^{-1} = T_n^{-1}(p)T_n^{-1}(h^2)T_n^{-1}(p) + R_3$. Because $\infty > M \geq h(x) \geq m > 0$, $T_n(h)$ and $T_n(h^2)$ are well-conditioned and can be approximated by circulant matrices C such that it holds: For each $\epsilon > 0$ there exist matrices E_5, E_6, E_7 and R_5, R_6, R_7 for which $\|E_j\|_2 \leq \epsilon$, $j = 5, 6, 7$ and R_j, $j = 5, 6, 7$ are matrices of low rank (the rank depends on ϵ and not on the dimension n) [2, 7] with

$$B_n = T_n(h) * T_n^{-1}(h^2) * T_n(h) + R_4 =$$
$$= T_n(h) * C_n^{-1}(h)C_n(h) * T_n^{-1}(h^2) * C_n(h)C_n^{-1}(h) * T_n(h) + R_4 =$$
$$= (I + E_5 + R_5) * (I + E_6 + R_6) * (I + E_7 + R_7) + R_4 = I + E + R . \qquad \square$$

THEOREM 3.8 (Well-conditioned Toeplitz Schur complement). *For uniformly well-conditioned spd Toeplitz Schur complements $S_n = T_n(f) - T_n^H(b)T_n^{-1}(g)T_n(b)$ with real f and $g \geq 0$ with $0 < |b(x)|^2/g(x) < \infty$, $f - |b|^2/g > 0$, all 2π-periodic continuous, the Toeplitz preconditioner $P_n = T_n(f(x) - |b(x)|^2/g(x))$ leads to a weakly clustered spectrum with eigenvalues uniformly bounded away from 0 and ∞. If $b(x)$ is real with zeros of even order the spectrum of the preconditioned Schur complement is strongly clustered around 1.*

Proof. All S_n and P_n are uniformly well-conditioned and the spectrum of $P_n^{-1}S_n$ is bounded in an interval $[1, M]$. With the following Theorem 3.9 this proves the first part of the Theorem. Furthermore, it holds

$$P_n^{-1} * S_n = T_n^{-1}(f - |b|^2/g) * (T_n(f) - T_n(b)^H T_n^{-1}(g)T_n(b)) =$$
$$= I + P_n^{-1} * (T_n(|b|^2/g) - T_n^H(b)T_n^{-1}(g)T_n(b)) .$$

If $b(x)$ has zeros, then $g(x)$ has the same zeros of double order. If b has only zeros of even order then we can write $b(x) = p(x)h_b(x)$ with a trigonometric polynomial $p(x)$. Furthermore, g can be written as $g(x) = p^2(x)h_g(x)$ with positive $h_b \geq m_b > 0$ and $h_g \geq m_g > 0$. Then, for real b it holds

$$T_n^H(b)T_n^{-1}(g)T_n(b) = T_n^H(ph_b)T_n^{-1}(p^2h_g)T_n(ph_b) = T_n(h_b)T_n(h_g)^{-1}T_n(h_b) + R$$

in view of Corollary 2.3. So we have to analyse only the case of well-conditioned $T_n(g)$ which can be treated like in the previous Theorem by using circulant approximations. $\square$

Next we consider ill-conditioned matrices. Here it turns out that for BT matrices the block circulant preconditioner can only ensure a weak clustering but no strong clustering. The proof of the weak clustering is based on the definition of approximating class of matrix sequences:

THEOREM 3.9 (Weak clustering of BC preconditioner for BT matrices, Theorem 3.1 in [16]). *For the Hermitian Toeplitz Schur complement of L^1 functions $S_n(f, g, b)$ it holds that the spectrum is distributed like the spectrum of the Toeplitz matrix $T_n(f - |b^2|/g)$. There-*

fore, the eigenvalues of the preconditioned Schur complement are weakly clustered around 1. *The same is true for related circulant preconditioners.*

THEOREM 3.10 (Counter example with no strong clustering). *For the Toeplitz Schur complement there exist examples, e.g., $f \in L^2$, where the above Toeplitz preconditioner from Theorem 3.9 that leads to a weak clustering, does not lead to a strong clustering.*

Proof. Consider the Schur complement $S_n = (T_n(p) + T_n(f^2)) - T_n(f)^2$ with a trigonometric polynomial like $p(x) = (1 - \cos(x))^m$ and function f with coefficients $t_j = 1/j$. Note that the sequence t_j is in l^2 and therefore the related Fourier series f is in L^2. The Toeplitz preconditioner is given by $T_n(p)$. Then it holds

$$T_n^{-1}(p) * S_n = I + T_n^{-1}(p) * (T_n(f^2) - T_n(f)^2))$$
$$(3.1) \qquad\qquad = I + T_n^{-1}(p) * (P_n H(f)H(f)P_n + Q_n H(f)H(f)Q_n) .$$

Here, $H(f)$ is the infinite Hilbert matrix. Because of Theorem 2.5 the eigenvalues, and therefore also the singular values are not clustered, and therefore also the eigenvalues of $T_n^{-1}(p)S_n$ are not clustered around 1 but each cluster leads to $O(\log(n))$ outliers. ☐

THEOREM 3.11 (Counter example for Toeplitz Schur complement preconditioner with unbounded norm). *For the Toeplitz Schur complement $S_n = A_n + T_n(f^2) - T_n(f)T_n(f)$ with Toeplitz matrices A_n there exists an example where the Toeplitz peconditioner that leads to a weak clustering following Theorem 3.9 has unbounded spectrum of the preconditioned system, e.g., for $f \in L^2$.*

Proof. Define the skewcirculant matrix $A_n = toeplitz(2, -1, 0, ...0, , 1)$ and $f(x)$ with coefficients $t_j = q^j$ with related Hankel matrix coefficients q^j. (Here we use the MATLAB-notation $T = toeplitz(x)$ to denote the symmetric Toeplitz matrix generated by vector x). With the eigenvectors u_j of A_n, relative to the standard eigendecomposition to A_n based on the Fourier matrix, we consider the Rayleigh quotients $u_j^H A_n u_j$ and $u_j^H H_n u_j$. It can be shown by direct computation that it holds $u_j^H H_j u_j = O(1/n)$. Therefore, for the eigenvector to small eigenvalues of A_n it holds $u_j^H A_h u_j = O(1/n^2)$, and the Rayleigh quotient of $u_j^H(A_n + H_n)u_j/u_j^H A_n u_j$ is unbounded. ☐

THEOREM 3.12. *For the normal equations $T_n(f)^2$ the Toeplitz preconditioner $T_n(f^2)$ from Theorem 3.9 guarantees only a weakly clustered spectrum, e.g., for real $f \in L^2$.*

Proof. Consider $f(x) \geq 0$ with coefficients $t_j = 1/j$, $j = 1, 2, \ldots$; $T_n(f)^2$ preconditioned by $T_n(f^2)$ leads to

$$I - T_n^{-1}(f^2) * T_n^2(f) = T_n^{-1}(f^2) * (T_n(f^2) - T_n^2(f)) =$$
$$(3.2) \qquad\qquad = T_n^{-1}(f) * (P_n H(f)H(f)P_n + Q_n H(f)H(f)Q_n)$$

and $O(\log(n))$ outliers in view of Theorem 2.5. ☐

Finally, let us summarize the clustering results on preconditioning multilevel and block Toeplitz matrices by multilevel or block circulant preconditioners:

1. For m-level Toeplitz matrices with equispaced grid, blocksize n, and total size $N = n^m$ there may be $O(N^{(m-1)/m}) = n^{m-1}$ outliers (this includes also the scalar Toeplitz case with $O(1)$ outliers and the 2-level case with $N = n^2$ and $O(n) = O(\sqrt{N})$ outliers).

2. For a BT matrix of size $N = k * n$, with fixed k, there may be $O(\log(N)) = O(\log(n))$ outliers in the ill-conditioned case.

So, in the ill-conditioned case for scalar Toeplitz matrices we get strong clustering while for BT and m-level Toeplitz matrices we get only a weak one. Nevertheless, the pcg method for BT systems converges much faster ($O(\log(N))$ outliers) than the one for m-level Toeplitz systems ($O(N^{(m-1)/m})$ outliers).

4. Finding efficient preconditioners for BT matrices and Toeplitz Schur Complements. An important class of preconditioners for scalar and multilevel Toeplitz matrices is given by trigonometric polynomials, resp. band Toeplitz matrices. A polynomial BT matrix is defined as a matrix with generating function whose entries are trigonometric polynomials. Unfortunately, given an ill-conditioned BT matrix it is not obvious whether one can find a spectral equivalent trigonometric polynomial BT matrix. So for the three examples

$$F_1(x) = \begin{pmatrix} x^2 & x \\ x & 1 + x^2 \end{pmatrix} \; , \; F_2(x) = \begin{pmatrix} x^2 & |x| \\ |x| & 1 + x^2 \end{pmatrix} \; , \; F_3(x) = \begin{pmatrix} x^2 + \rho|x|^5 & x \\ x & 1 + x^2 \end{pmatrix}$$
(4.1)

with small $\rho > 0$, the polynomial BT matrix

(4.2) $$P(x) = \begin{pmatrix} 2(1 - \cos(x))) & \sin(x) \\ \sin(x) & 1 + 2(1 - \cos(x))) \end{pmatrix} \geq 0$$

is spectral equivalent to F_1 and F_3, but for F_2 we cannot find a spectral equivalent polynomial. Note, that F_1 and F_2 have the same determinant, trace, and eigenvalues.

In the following, we present a recipe to define a trigonometric polynomial BT matrix for given $F(x)$. For simplicity we assume that $F(x)$ has $x_0 = 0$ as only singularity. First, we compute $\det(F(x))$ and assume that at $x_0 = 0$ it allows the expansion $\det(F(x)) = c\,x^m + O(|x|^{m+1})$. We split the partial functions $f_{ij}(x)$ of $F(x)$ into $f_{ij}(x) = fd_{ij}(x) + fn_{ij}(x)$ with $fd_{ij}(x)$ differentiable up to order m and $fn_{ij}(x) = O(|x|^{m+1})$ not necessarily differentiable at x_0. Then, we can reduce the partial function $fd_{ij}(x)$ to the coefficients $1, x^1, \ldots, x^{l_{ij}}$ that give a contribution to the leading term x^m in $\det(F(x))$. In fd_{ij} we can replace the occuring terms x^r, $r = 0, \ldots, l_{ij}$ by trigonometric polynomials of the form $\sin(x)^r$ or $(2 - 2\cos(x))^{r/2}$. In this way we can define a trigonometric polynomial BT matrix where $\det(P(x))$ has the same singularity as $\det(F(x))$. If the resulting polynomial has no other singularity and is positive definite it may lead to a spectral equivalent preconditioner. We can prove the following result.

THEOREM 4.1. *Let $F(x)$ be the generating matrix function for an spd ill-conditioned BT matrix with singularity at $x_0 = 0$. The determinant of $F(x)$ at $x_0 = 0$ is assumed to be of the form $\det(F(x)) = c\,x^m + O(|x|^{m+1})$. Suppose that we have found a trigonometric matrix polynomial $P(x)$ such that all the scalar functions $d_{ij}(x)$ in $D(x) = F(x) - P(x)$ are approximated at 0 such that $d_{ij}(x) = c_{ij}\,x^m + O(|x|^{m+1})$. Furthermore assume that $P(x)$ is spd and $P(x) > 0$ for $x \neq 0$. Then the spectrum of the preconditioned system $T_n^{-1}(P)T_n(F)$ is uniformly bounded away from 0 and ∞.*

Proof. Note, that $\det(P(x)) = \det(F(x)) + O(|x|^{m+1})$ near 0. The entries of $P^{-1}(x) * (F(x) - P(x))$ are also bounded near $x_0 = 0$ because $\det(P(x)) = c\,x^m + O(|x|^{m+1})$. Therefore, the eigenvalues of the preconditioned system $P^{-1}(x)F(x)$ are bounded from above. Furthermore, $P^{-1}(x)F(x) > 0$ for all x. $\qquad \square$

Note that the inverse of $F(x)$ can be written as $F^{-1}(x) = F(x)^\sharp / \det(F(x))$. With this notation the condition in Theorem 4.1 can be formulated in the form that for $P(x)$ all entries of the matrix $G := F(x)^\sharp D(x)$ have to be of the form $G_{ij}(x) = g_j\,x^m + O(|x|^{m+1})$.

Now let us return to the general problem of preconditining ill-conditioned BT matrices or Toeplitz Schur complements. We are interested in BT matrices where the solution can be reduced to the solution of scalar Toeplitz systems.

THEOREM 4.2 (BT Schur complement I). *Given a BT matrix with $k = 2$. The solution of the BT system can be reduced to solving scalar Toeplitz systems if one of the Schur complements $S_n(g) := T_n(f) - T_n^H(b) * T_n^{-1}(g) * T_n(b)$ or $S_n(f) := T_n(g) - T_n(b) * T_n(f) * T_n^H(b)$ is well-conditioned. We call $S_n(g)$ and $S_n(f)$ dual Schur complements.*

Proof. This is a direct consequence that via (2.1) we can reduce the BT matrix to scalar Toeplitz matrices and one of the Schur complements. Furthermore, in view of Theorem 3.8 we have efficient preconditinoers for well-conditioned Toeplitz Schur complements.   □

Note that for ill-conditioned 2×2 BT matrix one of the Schur complements may be ill-conditioned and the other may be well-conditioned, e.g., $F(x) = \begin{pmatrix} x^2 & x/2 \\ x/2 & 1 \end{pmatrix}$.

THEOREM 4.3 (BT and Schur complement II). *Given the pair of dual Schur complements $S_n(f)$ and $S_n(g)$. Then the solution of $S_n(f)$ can be reduced to the solution of $S_n(g)$. Therefore, for ill-conditioned $S_n(f)$ we can find an efficient preconditioner if $S_n(g)$ is well-conditioned or if there exists an efficient preconditioner for $S_n(g)$.*

Proof. Again, the result follows from equation (2.1) and Theorem 3.8.   □

One example is

$$F(x) = \begin{pmatrix} f & p \\ p & p^2 \end{pmatrix}$$

with trigonometric polynomial p. Then for the Schur complement it holds

$$T_n(f) - T_n(p)T_n(p^2)^{-1}T_n(p) = T_n(f) - I + R,$$

in view of Corollary 2.3 with $T_n(p^2) = T_n(p)T_n(p) + R$.

THEOREM 4.4. *Given a BT matrix with generating matrix function $F(x)$ Lebesgue integrable that admits the factorization*

$$F(x) = L(x) * U(x)$$

with $L(x)$ a trigonometric matrix polynomial and $U(x)$ a triangular matrix or vice versa. Then the solution of $T_n(F)$ can be reduced to solving scalar Toeplitz systems and band matrices.

Proof. We consider a BT matrix in the form (1.2). In view of Corollary 2.4 the matrix $T_n(F)$ can - up to low rank - be transformed in the product of a band matrix and a triangular matrix with Toeplitz matrices on the main diagonal blocks.   □

One example is

$$F(x) = \begin{pmatrix} f(x) & b(x) \\ b(x) & b(x) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} * \begin{pmatrix} f - b & 0 \\ b & b \end{pmatrix}$$

with real f, b L^1 functions and the above Schur complement factorization according to (2.1).

THEOREM 4.5. *Given a BT matrix with generating matrix function $F(x)$ Lebesgue integrable that admits the factorization*

$$F(x) = U(x) * R(x) * V(x)$$

with $U(x)$ and $V(x)$ trigonometric matrix polynomials and $R(x)$ a triangular matrix. Then the solution of $T_n(F)$ can be reduced to solving scalar Toeplitz systems and band matrices.

Proof. We consider a BT matrix in the form (1.2). In view of Corollary 2.4 the matrix $T_n(F)$ can - up to low rank - be transformed in the product of a band matrix and a triangular matrix with Toeplitz matrices on the main diagonal blocks.   □

One example is

$$F(x) = \begin{pmatrix} f(x) & b(x) \\ b(x) & f(x) \end{pmatrix} = (1/2) \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} f+b & 0 \\ 0 & f-b \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

with f and b real L^1 functions.

TABLE 5.1
Number of eigenvalues of the circulant preconditioned well-conditioned BT system outside $[0.9, 1.1]$.

Size	2*10	2*20	2*40	2*80	2*160	2*320
outliers	9	5	5	5	5	5

TABLE 5.2
Number of eigenvalues of N_n outside $[0.9, 1.001]$ for Toeplitz preconditioned Toeplitz normal equations.

Size	10	20	40	80	160	320	640
outliers	2	2	2	2	2	2	2

5. Numerical Results. First, we present numerical examples related to the Theorems from sections 3 and 4.

EXAMPLE 5.1. Table 5.1 presents an example for Theorem 3.6 with optimal circulant preconditioner for BT matrix to

$$F(x) = \begin{pmatrix} 1 + |x|/\pi & |x|/\pi \\ |x|/\pi & 1 \end{pmatrix}$$

with $x \in [-\pi, \pi]$. The spectrum is clustered and the number of outliers is bounded.

EXAMPLE 5.2. Next we display Theorem 3.7. Table 5.2 shows the number of outliers for a Toeplitz preconditioned Toeplitz normal equations. The function $f(x) = x^2$ has zero of even order at 0 and we consider the matrix $N_n := T_n(x^2) * T_n^{-1}(x^4) * T_n(x^2)$ with $x \in [-\pi, \pi]$. Note, that N_n is spectral equivalent to matrix $T_n(x^2)^2$ preconditioned by $T_n(x^4)$.

EXAMPLE 5.3. Table 5.3 presents an example for Theorem 3.8 with strong clustering for the optimal circulant preconditioned well-conditioned dual Toeplitz Schur complements $S_1 = I + T_n(|x|) - T_n(|x|) * T_n(|x|)$ and $S_2 = I - T_n(|x|) * T_n^{-1}(1 + |x|) * T_n(|x|)$ with $x \in [-\pi, \pi]$.

EXAMPLE 5.4. Next we consider the strong clustering described by Theorem 3.8. Table 5.4 deals with the Toeplitz Schur complement $2I + T_n(x^2) - T_n(x^2) * T_n^{-1}(x^4) * T_n(x^2)$ preconditioned by $T_n(1 + x^2)$ with $x \in [-\pi, \pi]$.

EXAMPLE 5.5. Table 5.5 presents an example for Theorem 3.10 with Toeplitz preconditioner for Toeplitz Schur complement $T_n(p) + T_n(f^2) - T_n^2(f)$; the preconditioner is given by $T_n(p)$ with $f(x) = |x|$, $x \in [-\pi, \pi]$, and $p(x) = 2 - 2\cos(x)$, resp. $p(x) = 6 - 8\cos(x) + 2\cos(2x)$.

EXAMPLE 5.6. We display Theorem 3.10 by Table 5.6. For the Toeplitz Schur complement $A_n + T_n(f^2) - T_n^2(f)$ we choose the preconditioner A_n with $f(x) = |x|$ with $x \in [-\pi, \pi]$ and $A_n(p)$ the skewcirculant matrix given by the polynomial $p(x) = 2 - 2\cos(x)$, resp. $p(x) = 6 - 8\cos(x) + 2\cos(2x)$.

EXAMPLE 5.7. Table 5.7 presents an example for Theorem 4.1 with polynomial BT preconditioner $P(x)$ for the three BT matrices $F_1(x)$, $F_2(x)$, and $F_3(x)$ from (4.1) and (4.2). We see, that P leads to bounded spectrum when applied on F_1 or F_3.

EXAMPLE 5.8. We consider the matrix function $F = \begin{pmatrix} 1 & x \\ x & 2x^2 \end{pmatrix}$. The associated BT matrix generated by F is:

$$B_n(F) = \begin{pmatrix} I_n & T_n(x) \\ T_n^H(x) & 2T_n(x^2) \end{pmatrix}.$$

For the solution of the BT system

$$B_n(F)\mathrm{x} = b$$

TABLE 5.3
Number of eigenvalues outside $[0.99, 1.01]$ as example for strong clustering for well-conditioned Toeplitz Schur complement with circulant preconditioner.

Size	10	20	40	80	160	320	640
outliers S_1	3	2	2	2	2	2	2
outliers S_2	3	2	2	2	2	2	2

TABLE 5.4
Number of eigenvalues outside $[0.9, 1.001]$ as example for strong clustering for well-conditioned Toeplitz Schur complement with Toeplitz preconditioner.

Size	10	20	40	80	160	320	640
outliers	2	2	2	2	2	2	2

we choose as preconditioner the block band Toeplitz matrix:

$$\begin{pmatrix} I_n & T_n(\sin(x)) \\ T_n(\sin(x)) & 2T_n(2 - 2\cos(x)) \end{pmatrix}.$$

The Schur complements of the above BT matrix are

$$S_1 = I_n - (1/2) * T_n(x)^H * T_n(x^2)^{-1} * T_n(x),$$

which is well-conditioned in view of Theorem 3.1 and does not need any preconditioning, and

$$S_2 = 2T_n(x^2) - T_n(x)^H * T_n(x),$$

which is ill-conditioned and needs preconditioning. For this we choose the band Toeplitz preconditioner

$$T_n(2 - 2\cos(x)).$$

In Table 5.8 we give the number of iterations of the pcg method for various values of n and for using various preconditioners. Thereby, we use the following abbreviations:
BT: cg for block Toeplitz System,
BBT: Block band Toeplitz preconditioning for block Toeplitz System,
CBT: Block circulant preconditioning for block Toeplitz System,
WS: cg for well-conditioned Schur complement,
IS: cg for ill-conditioned Schur complement,
BIS: Band Toeplitz preconditioning ill-conditioned Schur complement, and
CIS: Circulant preconditioning for ill-conditioned Schur complement.

We have to remark that for this example we get only a weak clustering and not a strong clustering for the band Toeplitz preconditioned ill-conditioned Schur complement, since the Hankel matrix related to the function x is similar to the Hilbert matrix (Theorem 3.10). Hence, the number of iterations in the 7th column shows a logarithmic growth.
Since the dual Schur complement is well-conditioned we get a strong clustering for the block band Toeplitz preconditioner applied on the block Toeplitz system (Theorem 4.2). As a consequence, the number of iterations in the 3rd column tends to be constant.
For the circulant preconditioned matrix for the Schur complement as well as for the block circulant preconditioned matrix for the BT system we get only a weak clustering (Theorem 3.9).

TABLE 5.5
*Number of eigenvalues of outside $[0.9, 1.001]$ as an example for no strong clustering for Toeplitz precondi-
tioned Toeplitz Schur complement.*

Size	10	20	40	80	160	320	640	1280
outliers $toeplitz(2, -1, 0, \ldots)$	2	2	2	2	3	3	4	4
outliers $toeplitz(6, -4, 1, 0, \ldots)$	2	2	3	4	4	6	6	8

TABLE 5.6
Maximum eigenvalue as an example for unboundedness for Toeplitz preconditioned Toeplitz Schur complement.

Size	10	20	40	80	160	320	640	1280
λ_{max} for $toeplitz(2, -1, 0, \ldots)$	3.1	6.0	12.2	25.3	52.2	106.7	216.5	437.1
λ_{max} for $toeplitz(6, -4, 1, 0, \ldots)$	2.0E1	1.8E2	1.6E3	1.4E4	1.1E5	9.2E5	7.5E6	6.0E7

Therefore, the number of iterations in the 4th and 8th columns show logarithmic growth.

EXAMPLE 5.9. $F = \begin{pmatrix} 1 & x^2 \\ x^2 & 2x^4 \end{pmatrix}$, $T_n(F) = \begin{pmatrix} I_n & T_n(x^2) \\ T_n(x^2) & 2T_n(x^4) \end{pmatrix}$. We use as block
band Toeplitz preconditioner for the BT system the matrix:

$$\begin{pmatrix} I_n & T_n(2 - 2\cos(x)) \\ T_n(2 - 2\cos(x)) & 2T_n((2 - 2\cos(x))^2) \end{pmatrix}$$

and as band Toeplitz preconditioner for the ill-conditioned Schur complement the matrix:

$$T_n((2 - 2\cos(x))^2).$$

In Table 5.9 we give the number of iterations of pcg method as we have done in Table 5.8.
The meaning of "*" is that the number of iterations exceeds the dimension of the considered
matrix.

We get the same remarks as in the previous example except the band Toeplitz precondi-
tioned ill-conditioned Schur complement. Note, that the Hankel matrix related to the function
x^2 is a compact operator (Theorem 3.4, see also [1]). Consequently, the number of iterations
in the 7th column tends to be constant.

EXAMPLE 5.10. $F = \begin{pmatrix} x^2 & \frac{1}{2}x^2 \\ \frac{1}{2}x^2 & x^2 \end{pmatrix}$, $T_n(F) = \begin{pmatrix} T_n(x^2) & \frac{1}{2}T_n(x^2) \\ \frac{1}{2}T_n(x^2) & T_n(x^2) \end{pmatrix}$. We use as
block band Toeplitz preconditioner for the BT system the matrix:

$$\begin{pmatrix} T_n(2 - 2\cos(x)) & T_n(1 - \cos(x)) \\ T_n(1 - \cos(x)) & T_n(2 - 2\cos(x)) \end{pmatrix}.$$

Both Schur complements are the same Toeplitz matrix: $\frac{3}{4}T_n(x^2)$, so we use as band Toeplitz
preconditioner for the ill-conditioned Schur complement the matrix:

$$\frac{3}{4}T_n(2 - 2\cos(x)).$$

This example is a special case of Theorem 4.5, so F can be written in the form

$$F(x) = (1/2)\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \frac{3}{2}x^2 & 0 \\ 0 & \frac{3}{2}x^2 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

TABLE 5.7

Minimum and maximum eigenvalue of the preconditioned spectrum $T_n^{-1}(P) * T_n(F_j)$, $j = 1, 2, 3$.

Size	10	20	40	80	160	320	640
$\lambda_{min}, \lambda_{max}$ for F_1	0.83,2.4	0.81,2.6	0.80,2.7	0.80,2.9	0.80,2.9	0.80,2.9	0.80,3.0
$\lambda_{min}, \lambda_{max}$ for F_2	0.1,9.0	4E-2,26.9	1E-2,96.5	4E-3,4E2	1E-3,1E3	4E-4,6E3	1E-4,2E4
$\lambda_{min}, \lambda_{max}$ for F_3	0.90,8.0	0.84,8.9	0.82,9.4	0.81,9.8	0.80,9.9	0.80,10.1	0.80,10.1

TABLE 5.8

Iterations for BT system and for Schur Complements of example 5.8

n	BT	BBT	CBT	WS	IS	BIS	CIS
4	8	7	5	2	2	2	2
8	15	10	12	3	4	4	4
16	31	12	14	3	8	8	5
32	64	14	15	3	17	9	5
64	128	14	16	3	39	10	6
128	202	14	16	3	86	11	6
256	350	14	18	3	187	11	6
512	619	13	19	4	395	12	9
1024	1189	13	20	4	819	12	10

Theorem 4.5 is applied, which means that the problem is reduced to solve the scalar Toeplitz system of the matrix $T_n(x^2)$. This system is efficiently solved by band Toeplitz preconditioned method to get superlinear convergence. Since F could be written also as the product:

$$F(x) = \begin{pmatrix} x^2 & 0 \\ 0 & x^2 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix},$$

where the first factor is a diagonal matrix function with roots of even order and the second one is a constant positive definite matrix function, we can use efficiently the block band diagonal Toeplitz preconditioner

$$D(x) = \begin{pmatrix} T_n(2 - 2\cos(x)) & 0 \\ 0 & T_n(2 - 2\cos(x)) \end{pmatrix}.$$

In Table 5.10 we give the associated numbers of iterations for all the methods mentioned above, where the column named by BBDT corresponds to the block band diagonal Toeplitz preconditioner. We get superlinearity in all preconditioned methods which confirms the validity of Theorem 4.5.

It should be mentioned here that the block band diagonal Toeplitz preconditioner for this example could be obtained also by Theorem 3.1 of [12], as an analogous preconditioner has been obtained in the Example 4.2 of the same paper.

6. Conclusions. We have characterized different methods to reduce the solution of BT matrices or Toeplitz Schur complements to the solution of scalar Toeplitz matrices. Furthermore, we have developed different preconditioning methods for block Toeplitz matrices and Toeplitz Schur complement matrices. In ill-conditioned cases we have to reckon with $O(\log(n))$ outliers and growing iteration count with increasing n. Furthermore, we have developed results on the spectrum of preconditioned BT matrices and Toeplitz Schur complements. We have shown that for some cases neither circulant preconditioner nor banded

TABLE 5.9
Iterations for BT system and for Schur Complements of example 5.9

n	BT	BBT	CBT	WS	IS	BIS	CIS
4	4	4	3	2	2	2	2
8	11	7	6	2	4	4	4
16	25	9	9	2	9	8	6
32	*	12	12	2	28	10	8
64	*	16	11	2	*	12	11
128	*	18	15	2	*	13	10
256	*	20	17	2	*	14	14
512	*	20	25	2	*	14	15
1024	*	20	24	2	*	14	24

TABLE 5.10
Iterations for BT system and for Schur Complements of example 5.10

n	BT	BBT	BBDT	IS	BIS
4	2	2	2	2	2
8	4	4	4	4	4
16	8	7	7	8	7
32	16	9	9	16	9
64	36	10	10	37	10
128	82	10	10	82	10
256	177	10	10	177	10
512	372	11	11	372	11
1024	768	11	11	768	11

preconditioner lead to an efficient iterative method. In such cases as alternative method the Multigrid approach for BT matrices [5] may be preferable, because these methods can also deal with zeros of uneven order in the generating function.

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