A FAMILY OF BLOCK PRECONDITIONERS FOR BLOCK SYSTEMS

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Abstract. We study the solution of block system $A_{mn}x = b$ by the preconditioned conjugate gradient method where A_{mn} is an m-by-m block matrix with n-by-n Toeplitz blocks. The preconditioner $c_F^{(1)}(A_{mn})$ is a matrix that preserves the block structure of A_{mn}. Specifically, it is defined to be the minimizer of $\|A_{mn} - C_{mn}\|_F$ over all m-by-m block matrices C_{mn} with n-by-n circulant blocks. We prove that if A_{mn} is positive definite, then $c_F^{(1)}(A_{mn})$ is positive definite too. We also show that $c_F^{(1)}(A_{mn})$ is a good preconditioner for solving separable block systems with Toeplitz blocks and quadrantally symmetric block Toeplitz systems. We then discuss some of the spectral properties of the operator $c_F^{(1)}$. In particular, we show that the operator norms $||c_F^{(1)}||_2 = ||c_F^{(1)}||_F = 1$.

Abbreviated Title. Block Preconditioners

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§1 Introduction.

Preconditioned conjugate gradient methods have been used efficiently in solving large matrix problems. The idea of using the method with circulant preconditioners for solving symmetric positive definite Toeplitz systems $T_n x = b$ was proposed by Strang [16] and Olkin [15] independently. The number of operations per iteration is of $O(n \log n)$ as circulant systems can be solved efficiently by fast Fourier transform (FFT) and the matrix-vector multiplication $T_n v$ can also be computed by the FFT by first embedding T_n into a $2n$-by-$2n$ circulant matrix. The convergence rate of the preconditioned conjugate gradient method depends on the whole spectrum of the preconditioned matrix. In general, the more clustered the eigenvalues are, the faster the convergence rate will be.

There are many circulant preconditioners that can produce clustered spectra, see Chan and Yeung [5]. One good example is T. Chan's [9] circulant preconditioner which is defined to be the minimizer of $\|T_n - C_n\|_F$ in Frobenius norm over all circulant matrices C_n. One can consider this circulant preconditioner from the operator point of view. Given any arbitrary n-by-n matrix A_n, we define an operator c_F which maps A_n to the matrix $c_F(A_n)$ that minimizes $\|A_n - C_n\|_F$ over all circulant matrices C_n. This circulant operator c_F has been studied in Chan, Jin and Yeung [3].

In this paper, we generalize the idea to the case of block matrices. Our interest is in solving systems $T_{mn}x = b$ where T_{mn} is an m-by-m block matrix with n-by-n Toeplitz blocks. This kind of systems occur in a variety of applications, such as the two-dimensional digital signal processing and the discretization of two-dimensional partial differential equations. Given such T_{mn}, we can use the mn-by-mn point-circulant matrix $c_F(T_{mn})$ as a circulant approximation to T_{mn}, see T. Chan and Olkin [10] and Chan and T. Chan [8]. In this paper, however, we consider another approximation to T_{mn} that preserves the block structure. The approximation is an extending to the one proposed by T. Chan and Olkin [10]. We define the matrix $c_F^{(1)}(T_{mn})$ to be the minimizer of $\|T_{mn} - C_{mn}\|_F$ over all m-by-m block matrices C_{mn} with n-by-n circulant blocks. We will show that the operator $c_F^{(1)}$ is well-defined for all mn-by-mn complex matrices A_{mn}. Some properties of $c_F^{(1)}$ are then discussed. In particular, we prove that if A_{mn} is positive definite, then $c_F^{(1)}(A_{mn})$ is also positive definite. We also show that the operator $c_F^{(1)}$ has operator norms $||c_F^{(1)}||_2 = ||c_F^{(1)}||_F = 1$.

We then consider the cost of using the preconditioned conjugate gradient method with the preconditioner $c_F^{(1)}(A_{mn})$ for solving block systems $A_{mn}x = b$. The convergence rate of the method is then analyzed for two specific types of block systems. The first one is the quadrantally symmetric block Toeplitz systems. We show that in this case, if the generating sequence of the matrices is absolutely summable, then the method converges in at most $O(\min\{m,n\})$ steps. Next we consider block matrices that are of the form $A_m \otimes T_n$ where A_m is nonsingular and T_n is a Toeplitz matrix with a positive 2π-periodic continuous generating function. We show that the resulting preconditioned system has spectrum clustered around 1 and hence the method converges superlinearly. Our numerical experiments have shown that $c_F^{(1)}(A_{mn})$ is indeed a good preconditioner for solving these block systems – the number of iterations is roughly a constant in both cases.

The outline of the paper is as follows. In §2, we first recall some properties of the point-circulant operator c_F. Then we introduce three different possible block preconditioners that preserve the block structure of the given matrix. In §3, we consider the cost of using $c_F^{(1)}(A_{mn})$ as a preconditioner for solving block systems $A_{mn}x = b$. The convergence rate of the method is analysed in §4 and numerical results are then given in §5.

§2 Operators for Block Matrices.

Let us begin by introducing the operator for point matrices. Given an n-by-n unitary matrix U, let

$$\mathcal{M}_U = \{U^*\Lambda_n U \mid \Lambda_n \text{ is an } n\text{-by-}n \text{ complex diagonal matrix}\},$$

where "$*$" denotes the conjugate transposition. We note that when U is equal to the

Fourier matrix F, $\mathcal{M}_F$ is the set of all circulant matrices, see Davis [11]. Let $\delta(A_n)$ denote the diagonal matrix whose diagonal is equal to the diagonal of the matrix A_n. The following Lemma was first proved by Chan, Jin and Yeung [3] for the case $U = F$ and was extended to the general unitary case by Huckle [13].

Lemma 1. *Let A_n be an arbitrary n-by-n matrix and $c_U(A_n)$ be the minimizer of $\|W_n - A_n\|_F$ over all $W_n \in \mathcal{M}_U$. Then*

(i) *$c_U(A_n)$ is uniquely determined by A_n and is given by*

$$c_U(A_n) = U^* \delta(U A_n U^*) U \ . \tag{1}$$

(ii) *If A_n is Hermitian, then so is $c_U(A_n)$. Furthermore, if $\lambda_{\min}(\cdot)$ and $\lambda_{\max}(\cdot)$ denote the largest and the smallest eigenvalues respectively, then we have*

$$\lambda_{\min}(A_n) \le \lambda_{\min}\big(c_U(A_n)\big) \le \lambda_{\max}\big(c_U(A_n)\big) \le \lambda_{\max}(A_n) \ .$$

In particular, if A_n is positive definite, then $c_U(A_n)$ is also positive definite.

(iii) *The operator c_U is a linear projection operator from the set of all n-by-n complex matrices into $\mathcal{M}_U$ and has the operator norms*

$$||c_U||_2 = \sup_{||A_n||_2=1} ||c_U(A_n)||_2 = 1$$

and

$$||c_U||_F = \sup_{||A_n||_F=1} ||c_U(A_n)||_F = 1.$$

(iv) When U is the n-by-n Fourier matrix F,

$$c_F(A_n) = \sum_{j=0}^{n-1} \Big(\frac{1}{n} \sum_{p-q\equiv j \pmod n} a_{pq}\Big) Q^j \ , \tag{2}$$

where Q is the n-by-n circulant matrix

$$Q \equiv \begin{bmatrix} 0 & & & & 1 \\ 1 & 0 & & & \\ 0 & 1 & \ddots & & \\ \vdots & & \ddots & \ddots & \\ 0 & & & 1 & 0 \end{bmatrix}. \tag{3}$$

The circulant matrix $c_F(A_n)$, first proposed by T. Chan [9], is a good preconditioner for solving some Toeplitz systems by the preconditioned conjugate gradient method, see Chan [6]. In the following, we call c_U the point-operator in order to distinguish it from the block-operators that we now introduce.

§2.1 Block-Operator $c_U^{(1)}$.

Let us now consider a general system $A_{mn}x = b$ where A_{mn} is an mn-by-mn matrix partitioned as

$$A_{mn} = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,m} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,m} \\ \vdots & \ddots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,m} \end{bmatrix}. \tag{4}$$

Here the blocks $A_{i,j}$ are square matrices of order n. We emphasize that we are interested in solving block systems where the blocks $A_{i,j}$ are Toeplitz matrices. In view of the point case, a natural choice of preconditioner for A_{mn} is

$$E_{mn} = \begin{bmatrix} c_F(A_{1,1}) & c_F(A_{1,2}) & \cdots & c_F(A_{1,m}) \\ c_F(A_{2,1}) & c_F(A_{2,2}) & \cdots & c_F(A_{2,m}) \\ \vdots & \ddots & \ddots & \vdots \\ c_F(A_{m,1}) & c_F(A_{m,2}) & \cdots & c_F(A_{m,m}) \end{bmatrix},$$

where the blocks $c_F(A_{i,j})$ are just the point-circulant approximations to $A_{i,j}$, see (2). We will show in §4 and §5 that E_{mn} is a good preconditioner for solving some block systems. In the following, however, we first study some of the spectral properties of the matrix E_{mn}.

Let $\delta^{(1)}(A_{mn})$ be defined by

$$\delta^{(1)}(A_{mn}) \equiv \begin{bmatrix} \delta(A_{1,1}) & \delta(A_{1,2}) & \cdots & \delta(A_{1,m}) \\ \delta(A_{2,1}) & \delta(A_{2,2}) & \cdots & \delta(A_{2,m}) \\ \vdots & \ddots & \ddots & \vdots \\ \delta(A_{m,1}) & \delta(A_{m,2}) & \cdots & \delta(A_{m,m}) \end{bmatrix}, \tag{5}$$

where each block $\delta(A_{i,j})$ is the diagonal matrix of order n whose diagonal is equal to the diagonal of the matrix $A_{i,j}$. The following Lemma gives the relation between $\sigma_{\max}(A_{mn})$ and $\sigma_{\max}\big(\delta^{(1)}(A_{mn})\big)$ where $\sigma_{\max}(\cdot)$ denotes the largest singular value.

Lemma 2. *Given any mn-by-mn complex matrix A_{mn} partitioned as in (4), we have*

$$\sigma_{\max}\left(\delta^{(1)}(A_{mn})\right) \le \sigma_{\max}(A_{mn}). \tag{6}$$

Furthermore, when A_{mn} is Hermitian, we have

$$\lambda_{\min}(A_{mn}) \le \lambda_{\min}\left(\delta^{(1)}(A_{mn})\right) \le \lambda_{\max}\left(\delta^{(1)}(A_{mn})\right) \le \lambda_{\max}(A_{mn}) \ . \tag{7}$$

In particular, if A_{mn} is positive definite, then $\delta^{(1)}(A_{mn})$ is also positive definite.

Proof. Let $(A_{mn})_{i,j;k,l} = (A_{k,l})_{ij}$ be the (i,j)th entry of the (k,l)th block of A_{mn}. Let P be the permutation matrix that satisfies

$$(P^* A_{mn} P)_{k,l;i,j} = (A_{mn})_{i,j;k,l}, \quad 1 \le i,j \le n, 1 \le k,l \le m. \tag{8}$$

Then it is easy to see that $B_{mn} \equiv P^* \delta^{(1)}(A_{mn}) P$ is of the form

$$B_{mn} = \begin{bmatrix} B_{1,1} & 0 & \cdots & 0 \\ 0 & B_{2,2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{n,n} \end{bmatrix} .$$

Clearly the matrices B_{mn} and $\delta^{(1)}(A_{mn})$ have the same singular values and eigenvalues. For each k, since $B_{k,k}$ is a principal submatrix of the matrix A_{mn}, it follows that

$$\sigma_{\max}(B_{k,k}) \le \sigma_{\max}(A_{mn}),$$

see for instance, Thompson [17]. Hence we have

$$\sigma_{\max}\left(\delta^{(1)}(A_{mn})\right) = \sigma_{\max}(B_{mn}) = \max_k \left(\sigma_{\max}(B_{k,k})\right) \le \sigma_{\max}(A_{mn}) \ .$$

When A_{mn} is Hermitian, by Cauchy's Interlace Theorem, see Golub and van Loan [12], we then have

$$\begin{aligned} \lambda_{\min}(A_{mn}) \le & \min_k \left(\lambda_{\min}(B_{k,k})\right) = \lambda_{\min}\left(\delta^{(1)}(A_{mn})\right) \\ \le & \lambda_{\max}\left(\delta^{(1)}(A_{mn})\right) = \max_k \left(\lambda_{\max}(B_{k,k})\right) \le \lambda_{\max}(A_{mn}) \ . \quad \square \end{aligned}$$

In the following, we use $\mathcal{D}^{(1)}_{m,n}$ to denote the set of all m-by-m block matrices where each block is a complex diagonal matrix of order n, i.e. $\mathcal{D}^{(1)}_{m,n}$ is the set of all matrices of the form given by (5). Let

$$\mathcal{M}^{(1)}_U = \{(I \otimes U)^* \Lambda^{(1)}_{mn} (I \otimes U) \mid \Lambda^{(1)}_{mn} \in \mathcal{D}^{(1)}_{m,n}\} ,$$

where I is the m-by-m identity matrix and U is any given n-by-n unitary matrix. We then define the operator $c^{(1)}_U$ to be the mapping that maps every mn-by-mn matrix A_{mn} to the minimizer of $\|W_{mn} - A_{mn}\|_F$ over all $W_{mn} \in \mathcal{M}^{(1)}_U$. Some of the properties of this operator are given in the following Theorem.

Theorem 1. *For any arbitrary mn-by-mn complex matrix A_{mn} partitioned as in (4), let $c^{(1)}_U(A_{mn})$ be the minimizer of $\|W_{mn} - A_{mn}\|_F$ over all $W_{mn} \in \mathcal{M}^{(1)}_U$. Then*

(i) *$c^{(1)}_U(A_{mn})$ is uniquely determined by A_{mn} and is given by*

$$c^{(1)}_U(A_{mn}) = (I \otimes U)^* \delta^{(1)} \left[(I \otimes U) A_{mn} (I \otimes U)^*\right] (I \otimes U). \tag{9}$$

(ii) *$c^{(1)}_U(A_{mn})$ is also given by*

$$c^{(1)}_U(A_{mn}) = \begin{bmatrix} c_U(A_{1,1}) & c_U(A_{1,2}) & \cdots & c_U(A_{1,m}) \\ c_U(A_{2,1}) & c_U(A_{2,2}) & \cdots & c_U(A_{2,m}) \\ \vdots & \ddots & \ddots & \vdots \\ c_U(A_{m,1}) & c_U(A_{m,2}) & \cdots & c_U(A_{m,m}) \end{bmatrix}, \tag{10}$$

where c_U is the point-operator defined by (1).

(iii) *We have*

$$\sigma_{\max}\left(c^{(1)}_U(A_{mn})\right) \leq \sigma_{\max}(A_{mn}). \tag{11}$$

(iv) *If A_{mn} is Hermitian, then $c^{(1)}_U(A_{mn})$ is also Hermitian and*

$$\lambda_{\min}(A_{mn}) \leq \lambda_{\min}\left(c^{(1)}_U(A_{mn})\right) \leq \lambda_{\max}\left(c^{(1)}_U(A_{mn})\right) \leq \lambda_{\max}(A_{mn}) .$$

In particular, if A_{mn} is positive definite, then $c^{(1)}_U(A_{mn})$ is also positive definite.

(v) *The operator $c^{(1)}_U$ is a linear projection operator from the set of all mn-by-mn complex matrices into $\mathcal{M}^{(1)}_U$ and has the operator norms*

$$\|c^{(1)}_U\|_2 \equiv \sup_{\|A_{mn}\|_2 = 1} \|c^{(1)}_U(A_{mn})\|_2 = 1$$

and

$$\|c_U^{(1)}\|_F \equiv \sup_{\|A_{mn}\|_F=1} \|c_U^{(1)}(A_{mn})\|_F = 1.$$

Proof.

(i) Let $W_{mn} \in \mathcal{M}_U^{(1)}$ be given by

$$W_{mn} = (I \otimes U)^* \Lambda_{mn}^{(1)} (I \otimes U) \ ,$$

where $\Lambda_{mn}^{(1)} \in \mathcal{D}_{m,n}^{(1)}$. Since the Frobenius norm is unitary invariant, we have

$$\begin{aligned} \|W_{mn} - A_{mn}\|_F =& \|(I \otimes U)^* \Lambda_{mn}^{(1)} (I \otimes U) - A_{mn}\|_F \\ =& \|\Lambda_{mn}^{(1)} - (I \otimes U) A_{mn} (I \otimes U)^*\|_F \ . \end{aligned}$$

Thus the problem of minimizing $\|W_{mn} - A_{mn}\|_F$ over $\mathcal{M}_U^{(1)}$ is equivalent to the problem of minimizing $\|\Lambda_{mn}^{(1)} - (I \otimes U) A_{mn} (I \otimes U)^*\|_F$ over $\mathcal{D}_{m,n}^{(1)}$. Since $\Lambda_{mn}^{(1)}$ can only affect the diagonal of each block of $(I \otimes U) A_{mn} (I \otimes U)^*$, we see that the solution for the latter problem is $\Lambda_{mn}^{(1)} = \delta^{(1)}\left[(I \otimes U) A_{mn} (I \otimes U)^*\right]$. Hence

$$c_U^{(1)}(A_{mn}) = (I \otimes U)^* \delta^{(1)}\left[(I \otimes U) A_{mn} (I \otimes U)^*\right] (I \otimes U)$$

is the minimizer of $\|W_{mn} - A_{mn}\|_F$. It is clear that $\Lambda_{mn}^{(1)}$ and hence $c_U^{(1)}(A_{mn})$ are uniquely determined by A_{mn}.

(ii) Since

$$\delta^{(1)}\left[(I \otimes U) A_{mn} (I \otimes U)^*\right] = \begin{bmatrix} \delta(UA_{1,1}U^*) & \delta(UA_{1,2}U^*) & \cdots & \delta(UA_{1,m}U^*) \\ \delta(UA_{2,1}U^*) & \delta(UA_{2,2}U^*) & \cdots & \delta(UA_{2,m}U^*) \\ \vdots & \ddots & \ddots & \vdots \\ \delta(UA_{m,1}U^*) & \delta(UA_{m,2}U^*) & \cdots & \delta(UA_{m,m}U^*) \end{bmatrix} ,$$

by (1) and (9), we see that $c_U^{(1)}(A_{mn})$ is also given by (10).

(iii) For general mn-by-mn matrix A_{mn}, we have by (9) and (6)

$$\begin{aligned} \sigma_{\max}\big(c_U^{(1)}(A_{mn})\big) =& \sigma_{\max}\left[\delta^{(1)}\big((I \otimes U) A_{mn} (I \otimes U)^*\big)\right] \\ \leq& \sigma_{\max}\left[(I \otimes U) A_{mn} (I \otimes U)^*\right] = \sigma_{\max}(A_{mn}) \ . \end{aligned}$$

(iv) If A_{mn} is Hermitian, then it is clear from (10) and Lemma 1 (ii) that $c_U^{(1)}(A_{mn})$ is also Hermitian. Moreover, by (7) and (9), we have

$$\begin{aligned}\lambda_{\min}(A_{mn}) =&\lambda_{\min}\left[(I\otimes U)A_{mn}(I\otimes U)^*\right]\\ \leq&\lambda_{\min}\left[\delta^{(1)}\left((I\otimes U)A_{mn}(I\otimes U)^*\right)\right]\\ =&\lambda_{\min}\left(c_U^{(1)}(A_{mn})\right)\leq\lambda_{\max}\left(c_U^{(1)}(A_{mn})\right)\\ =&\lambda_{\max}\left[\delta^{(1)}\left((I\otimes U)A_{mn}(I\otimes U)^*\right)\right]\\ \leq&\lambda_{\max}\left[(I\otimes U)A_{mn}(I\otimes U)^*\right]=\lambda_{\max}(A_{mn}) \ .\end{aligned}$$

(v) By (11), we have

$$\|c_U^{(1)}(A_{mn})\|_2=\sigma_{\max}[c_U^{(1)}(A_{mn})]\leq\sigma_{\max}(A_{mn})=\|A_{mn}\|_2.$$

However, for the mn-by-mn identity matrix I_{mn}, we have $\|c_U^{(1)}(I_{mn})\|_2=\|I_{mn}\|_2=1$. Hence $\|c_U^{(1)}\|_2=1$. For the Frobenius norm, we also have

$$\begin{aligned}\|c_U^{(1)}(A_{mn})\|_F&=\|\delta^{(1)}\left[(I\otimes U)A_{mn}(I\otimes U)^*\right]\|_F\\ &\leq\|(I\otimes U)A_{mn}(I\otimes U)^*\|_F=\|A_{mn}\|_F \ .\end{aligned}$$

Since $\|c_U^{(1)}(\frac{1}{\sqrt{mn}}I_{mn})\|_F=\frac{1}{\sqrt{mn}}\|I_{mn}\|_F=1$, it follows that $\|c_U^{(1)}\|_F=1$. $\square$

§2.2 Block-Operator $\tilde{c}_V^{(1)}$.

For matrices A_{mn} partitioned as in (4), we can define another block approximation to them. Let $\tilde{\delta}^{(1)}(A_{mn})$ be defined by

$$\tilde{\delta}^{(1)}(A_{mn})\equiv\begin{bmatrix}A_{1,1}&0&\cdots&0\\0&A_{2,2}&\cdots&0\\ \vdots&\ddots&\ddots&\vdots\\0&0&\cdots&A_{m,m}\end{bmatrix}. \tag{12}$$

In the following, we use $\tilde{\mathcal{D}}_{m,n}^{(1)}$ to denote the set of all m-by-m block diagonal matrices where each block is a complex matrix of order n, i.e. $\tilde{\mathcal{D}}_{m,n}^{(1)}$ is the set of all matrices of the form given by (12). Let

$$\tilde{\mathcal{M}}_V^{(1)}=\{(V\otimes I)^*\tilde{\Lambda}_{mn}^{(1)}(V\otimes I)\mid\tilde{\Lambda}_{mn}^{(1)}\in\tilde{\mathcal{D}}_{m,n}^{(1)}\}\ ,$$

where V is any given m-by-m unitary matrix and I is the n-by-n identity matrix.

We define the operator $\tilde{c}_V^{(1)}$ to be the mapping that maps every mn-by-mn matrix A_{mn} to the minimizer of $\|W_{mn} - A_{mn}\|_F$ over all $W_{mn} \in \tilde{\mathcal{M}}_V^{(1)}$. Similar to Theorem 1, we have the following Theorem.

Theorem 2. *For any arbitrary mn-by-mn complex matrix A_{mn} partitioned as in (4), let $\tilde{c}_V^{(1)}(A_{mn})$ be the minimizer of $\|W_{mn} - A_{mn}\|_F$ over all $W_{mn} \in \tilde{\mathcal{M}}_V^{(1)}$. Then*

(i) *$\tilde{c}_V^{(1)}(A_{mn})$ is uniquely determined by A_{mn} and is given by*

$$\tilde{c}_V^{(1)}(A_{mn}) = (V \otimes I)^* \tilde{\delta}^{(1)}\left[(V \otimes I) A_{mn} (V \otimes I)^*\right](V \otimes I). \tag{13}$$

(ii) *We have*

$$\sigma_{\max}\left(\tilde{c}_V^{(1)}(A_{mn})\right) \leq \sigma_{\max}(A_{mn}).$$

(iii) *If A_{mn} is Hermitian, then $\tilde{c}_V^{(1)}(A_{mn})$ is also Hermitian and*

$$\lambda_{\min}(A_{mn}) \leq \lambda_{\min}\left(\tilde{c}_V^{(1)}(A_{mn})\right) \leq \lambda_{\max}\left(\tilde{c}_V^{(1)}(A_{mn})\right) \leq \lambda_{\max}(A_{mn}) \ .$$

In particular, if A_{mn} is positive definite, then $\tilde{c}_V^{(1)}(A_{mn})$ is also positive definite.

(iv) *The operator $\tilde{c}_V^{(1)}$ is a linear projection operator from the set of all mn-by-mn complex matrices into $\tilde{\mathcal{M}}_V^{(1)}$ and has the operator norms*

$$\|\tilde{c}_V^{(1)}\|_2 = \|\tilde{c}_V^{(1)}\|_F = 1.$$

The proof of the Theorem is quite similar to that of Theorem 1, we therefore omit it. We note however that Theorem 2 (ii)-(iv) can be proved easily by using the following relationship between $c_U^{(1)}$ and $\tilde{c}_V^{(1)}$.

Lemma 3. *Let U be any given unitary matrix and P be the permutation matrix defined in (8). Then for any arbitrary mn-by-mn complex matrix A_{mn} partitioned as in (4), we have*

$$\delta^{(1)}(A_{mn}) = P\tilde{\delta}^{(1)}(P^* A_{mn} P)P^*$$

and

$$c_U^{(1)}(A_{mn}) = P\tilde{c}_U^{(1)}(P^*A_{mn}P)P^*.$$

Proof. To prove the first equality, we note that by the definition of $\tilde{\delta}^{(1)}$ and (8), we have

$$\begin{aligned}
[\tilde{\delta}^{(1)}(P^*A_{mn}P)]_{k,l;i,j} &= \begin{cases} (P^*A_{mn}P)_{k,l;i,j} & i = j \ , \\ 0 & i \neq j \ , \end{cases} \\
&= \begin{cases} (A_{mn})_{i,j;k,l} & i = j \ , \\ 0 & i \neq j \ . \end{cases}
\end{aligned}$$

Hence

$$[P\tilde{\delta}^{(1)}(P^*A_{mn}P)P^*]_{i,j;k,l} = [\tilde{\delta}^{(1)}(P^*A_{mn}P)]_{k,l;i,j} = \begin{cases} (A_{mn})_{i,j;k,l} & i = j \ , \\ 0 & i \neq j \ , \end{cases}$$

which by definition is equal to $[\delta^{(1)}(A_{mn})]_{i,j;k,l}$.

To prove the second equality, we first note that

$$(I \otimes U)P = P(U \otimes I)$$

for any matrix U. Hence by (13) and (9), we have

$$\begin{aligned}
P\tilde{c}_U^{(1)}(P^*A_{mn}P)P^* &= P(U \otimes I)^*\tilde{\delta}^{(1)}[(U \otimes I)P^*A_{mn}P(U \otimes I)^*](U \otimes I)P^* \\
&= (I \otimes U)^*P\tilde{\delta}^{(1)}[P^*(I \otimes U)A_{mn}(I \otimes U)^*P]P^*(I \otimes U) \\
&= (I \otimes U)^*\delta^{(1)}[(I \otimes U)A_{mn}(I \otimes U)^*](I \otimes U) = c_U^{(1)}(A_{mn}). \quad \square
\end{aligned}$$

§2.3 Operator $c_{V,U}^{(2)}$.

Intuitively, $c_U^{(1)}(A_{mn})$ and $\tilde{c}_V^{(1)}(A_{mn})$ resemble the diagonalization of A_{mn} along one specific direction. It is then natural to consider the matrix that results from diagonalization along both directions. Thus let $c_{V,U}^{(2)}$ denote the composite of the two operators, i.e. $c_{V,U}^{(2)} \equiv \tilde{c}_V^{(1)} \circ c_U^{(1)}$. The following Lemma will be used to derive the properties of the operator $c_{V,U}^{(2)}$.

Lemma 4. *For any given A_{mn} partitioned as in (4), we have*

$$(I \otimes U)^* \tilde{\delta}^{(1)}(A_{mn})(I \otimes U) = \tilde{\delta}^{(1)}[(I \otimes U)^* A_{mn}(I \otimes U)] \ , \tag{14}$$

and

$$(V \otimes I)\delta^{(1)}(A_{mn})(V \otimes I)^* = \delta^{(1)}[(V \otimes I)A_{mn}(V \otimes I)^*] \ . \tag{15}$$

Furthermore,

$$\tilde{\delta}^{(1)} \circ \delta^{(1)}(A_{mn}) = \delta(A_{mn}) = \delta^{(1)} \circ \tilde{\delta}^{(1)}(A_{mn}) \ . \tag{16}$$

The proof of Lemma 4 is straightforward, we therefore omit it. By using Lemma 4, we can prove the following Theorem which states that the operator $c^{(2)}_{V,U}$ is just a particular case of the point-operator.

Theorem 3. *For any given A_{mn} partitioned as in (4), we have*

$$c^{(2)}_{V,U}(A_{mn}) = c_{V\otimes U}(A_{mn}) \ ,$$

where $c_{V\otimes U}$ is the point-operator defined in Lemma 1.

Proof. For any given A_{mn}, by definitions of $c^{(1)}_U$ and $\tilde{c}^{(1)}_V$, we have

$$\begin{aligned}
& c^{(2)}_{V,U}(A_{mn}) \\
=& \tilde{c}^{(1)}_V[c^{(1)}_U(A_{mn})] \\
=& (V \otimes I)^* \tilde{\delta}^{(1)}\big\{(V \otimes I)\big[(I \otimes U)^* \delta^{(1)}[(I \otimes U)A_{mn}(I \otimes U)^*](I \otimes U)\big](V \otimes I)^*\big\}(V \otimes I) \\
=& (V \otimes I)^* \tilde{\delta}^{(1)}\big\{(I \otimes U)^*(V \otimes I)\delta^{(1)}[(I \otimes U)A_{mn}(I \otimes U)^*](V \otimes I)^*(I \otimes U)\big\}(V \otimes I).
\end{aligned}$$

Hence by (14), (15) and (16), we have

$$\begin{aligned}
c^{(2)}_{V,U}(A_{mn}) =& (V \otimes U)^* \tilde{\delta}^{(1)}\big\{[\delta^{(1)}[(V \otimes U)A_{mn}(V \otimes U)^*]\big\}(V \otimes U) \\
=& (V \otimes U)^* \delta[(V \otimes U)A_{mn}(V \otimes U)^*](V \otimes U) = c_{V\otimes U}(A_{mn}) \ . \quad \square
\end{aligned}$$

Since $c^{(2)}_{V,U}$ is just another point-operator, we therefore will concentrate our discussion on $c^{(1)}_U$ and $\tilde{c}^{(1)}_V$ in the remaining of the paper. We remark that $c^{(2)}_{V,U}(A_{mn})$ is an approximation of A_{mn} in two directions whereas $c^{(1)}_U(A_{mn})$ and $\tilde{c}^{(1)}_V(A_{mn})$ are approximations in one direction only (with the other direction being approximated exactly). Thus we expect that the $c_U^{(1)}(A_{mn})$ and $\tilde{c}_V^{(1)}(A_{mn})$ are better preconditioners than $c_{V,U}^{(2)}(A_{mn})$. This is confirmed by the numerical results in §5.

We now give two simple formula for finding $c_U^{(1)}(A_{mn})$ and $\tilde{c}_V^{(1)}(A_{mn})$ in the case where U and V are just the Fourier matrix F. When $U = F$, we have by (10),

$$c_F^{(1)}(A_{mn}) = \begin{bmatrix} c_F(A_{1,1}) & c_F(A_{1,2}) & \cdots & c_F(A_{1,m}) \\ c_F(A_{2,1}) & c_F(A_{2,2}) & \cdots & c_F(A_{2,m}) \\ \vdots & \ddots & \ddots & \vdots \\ c_F(A_{m,1}) & c_F(A_{m,2}) & \cdots & c_F(A_{m,m}) \end{bmatrix}, \tag{17}$$

where each block $c_F(A_{i,j})$ is T. Chan's circulant preconditioner for $A_{i,j}$.

Next we find $\tilde{c}_F^{(1)}(A_{mn})$ by using Lemma 3. We first let $A_{mn} = P^* B_{mn} P$ and partition B_{mn} into n^2 blocks with each block $B_{i,j}$ an m-by-m matrix. Then by Lemma 3 and (17), we have

$$[\tilde{c}_F^{(1)}(A_{mn})]_{i,j;k,l} = [P^* c_F^{(1)}(B_{mn})P]_{i,j;k,l} = [c_F^{(1)}(B_{mn})]_{k,l;i,j} = (c_F(B_{i,j}))_{kl},$$

where $B_{i,j}$ is the (i,j)th block of the matrix B_{mn}. By (2), we see that the (k,l)th entry of the circulant matrix $c_F(B_{i,j})$ is given by

$$(c_F(B_{i,j}))_{kl} = \frac{1}{m} \sum_{p-q \equiv k-l \pmod m} (B_{i,j})_{pq}.$$

Since $(B_{i,j})_{pq} = (A_{p,q})_{ij}$, we have

$$[\tilde{c}_F^{(1)}(A_{mn})]_{i,j;k,l} = \frac{1}{m} \sum_{p-q \equiv k-l \pmod m} (A_{p,q})_{ij}, \quad 1 \le i,j \le n, 1 \le k,l \le m.$$

Thus the (k,l)th block of $\tilde{c}_F^{(1)}(A_{mn})$ is given by $\frac{1}{m}\sum_{p-q\equiv k-l \pmod m}(A_{pq})$. Since it depends only on $k-l \pmod m$, we see that $\tilde{c}_F^{(1)}(A_{mn})$ is a block circulant matrix. Using the definition of the matrix Q in (3), we further have

$$\tilde{c}_F^{(1)}(A_{mn}) = \frac{1}{m} \sum_{j=0}^{m-1} (Q^j \otimes \sum_{p-q \equiv j \pmod m} A_{p,q}) \; .$$

§3 Block Preconditioners for Block Systems.

In this section, we consider the cost of solving block systems $A_{mn}x = b$ by the preconditioned conjugate gradient method with preconditioner $c_F^{(1)}(A_{mn})$. The analysis for $\tilde{c}_F^{(1)}(A_{mn})$ is similar. We first recall that in each iteration of the preconditioned conjugate gradient method, we have to compute the matrix-vector multiplication $A_{mn}v$ for some vector v and solve the system

$$c_F^{(1)}(A_{mn})y = d \ , \tag{18}$$

for some vector d, see Golub and van Loan [12].

§3.1 General Matrices.

Let A_{mn} be a general mn-by-mn matrix. We note that by (9), the solution to (18) is given by

$$y = (I \otimes F)^* \left[\delta^{(1)}\left((I \otimes F)A_{mn}(I \otimes F)^*\right)\right]^{-1}(I \otimes F)d \ . \tag{19}$$

Hence before we start the iteration, we should form the matrix

$$\Delta \equiv \delta^{(1)}\left((I \otimes F)A_{mn}(I \otimes F)^*\right)$$

and compute its inverse. We note that by (17), the (i,j)th block of Δ is just $Fc_F(A_{i,j})F^*$. By (1), $Fc_F(A_{i,j})F^* = \delta(FA_{i,j}F^*)$ and hence can be computed in n^2 operations and one FFT, see Chan, Jin and Yeung [3]. Thus the cost of obtaining Δ is $O(m^2n^2)$ operations. Next we compute its inverse.

We first permute the matrix Δ by P to obtain

$$B_{mn} = P^*\Delta P = \begin{bmatrix} B_{1,1} & 0 & \cdots & 0 \\ 0 & B_{2,2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{n,n} \end{bmatrix} .$$

We then compute the LU decompositions for all diagonal blocks $B_{k,k}$. That will take $O(nm^3)$ operations. Totally, it requires $O(n^2m^2 + nm^3)$ operations in the initialization step.

After obtaining the LU factors of Δ, we start the iteration. For a general dense matrix A_{mn}, $A_{mn}v$ can be computed in $O(n^2m^2)$. To get the vector y in (19), we note that by using the FFT, vectors of the form $(I \otimes F)d$ can be computed in $O(mn\log n)$ operations. Using the LU factors of Δ, $O(nm^2)$ operations are need to compute $\Delta^{-1}d$ for any vector d. Totally, the cost per iteration is $O(mn\log n) + O(nm^2)$ operations.

Thus the algorithm for solving system $A_{mn}x = b$ for general matrix A_{mn} requires $O(n^2m^2 + nm^3)$ operations in the initialization step and $O(n^2m^2)$ operations per iteration. Clearly if A_{mn} is sparse, the cost can be reduced. We will consider, in the next two subsections, two types of block systems where the cost can be drastically reduced.

Finally, we note that some of the block operations mentioned above can be done parallelly. For instance, the diagonal $\delta(FA_{i,j}F^*)$ of the blocks $c_F(A_{i,j})$ can be obtained in $O(n^2)$ parallel steps with $O(m^2)$ processors and the LU decompositions of the blocks B_{kk} in B_{mn} can also be computed in parallel. This can further reduce the cost per iteration.

§3.2 Quadrantally Symmetric Block Toeplitz Matrices.

Let us consider the family of block Toeplitz systems $T_{mn}x = b$ where T_{mn} is of the form

$$T_{mn} = \begin{bmatrix} T_{1,1} & T_{1,2} & \cdots & T_{1,m} \\ T_{2,1} & T_{2,2} & \cdots & T_{2,m} \\ \vdots & \ddots & \ddots & \vdots \\ T_{m,1} & T_{m,2} & \cdots & T_{m,m} \end{bmatrix} = \begin{bmatrix} T_{(0)} & T_{(1)} & \cdots & T_{(m-1)} \\ T_{(1)} & T_{(0)} & \cdots & T_{(m-2)} \\ \vdots & \ddots & \ddots & \vdots \\ T_{(m-1)} & T_{(m-2)} & \cdots & T_{(0)} \end{bmatrix}. \tag{20}$$

Here the blocks $T_{i,j} = T_{(|i-j|)}$ are themselves symmetric Toeplitz matrices of order n. Such T_{mn} are called quadrantally symmetric block Toeplitz matrices.

By (17), the blocks of $c_F^{(1)}(T_{mn})$ are just $c_F(T_{(k)})$. Hence by (2) and the fact that $T_{(k)}$ is Toeplitz, the diagonal $\delta(FT_{(k)}F^*)$ can be computed in $O(n\log n)$ operations. Therefore, we need $O(mn\log n)$ operations to form $\Delta = \delta^{(1)}\big((I \otimes F)T_{mn}(I \otimes F)^*\big)$. We emphasize that in this case, there is no need to compute the LU factors of Δ. In fact,

$$P^*\Delta P = \begin{bmatrix} \tilde{T}_{1,1} & 0 & \cdots & 0 \\ 0 & \tilde{T}_{2,2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \tilde{T}_{n,n} \end{bmatrix},$$

where

$$(\tilde{T}_{k,k})_{ij} = \big(\delta(FT_{i,j}F^*)\big)_{kk} = \big(\delta(FT_{(|i-j|)}F^*)\big)_{kk}, \quad 1 \le i,j \le m, \quad 1 \le k \le n.$$

Hence we see that the diagonal blocks $\tilde{T}_{k,k}$ are still symmetric Toeplitz matrices of order m. Therefore it requires only $O(m \log^2 m)$ operations to compute $\tilde{T}_{k,k}^{-1} v$ for any vector v, see Ammar and Gragg [1]. Thus the system $c_F^{(1)}(T_{mn})y = d$ can be solved in $O(nm \log^2 m)$ operations.

Next we consider the cost of the matrix-vector multiplication $T_{mn}v$. We recall that for any Toeplitz matrix $T_{(k)}$, the matrix vector multiplication $T_{(k)}w$ can be computed by the FFT by first embedding $T_{(k)}w$ into a $2n$-by-$2n$ circulant matrix and extending w to a $2n$-vector by zeros. For the matrix-vector product $T_{mn}v$, we can use the same trick. We first embed T_{mn} into a (blockwise) $2m$-by-$2m$ block circulant matrix where each block itself is a $2n$-by-$2n$ circulant matrix. Then we extend v to a $4mn$-vector by putting zeros in the appropriate places. Using FFT, or more precisely using $(F_{2m} \otimes F_{2n})$ to diagonalize the $2m$-by-$2m$ block circulant matrix, we see that $T_{mn}v$ can be obtained in $O(mn(\log m + \log n))$ operations.

Thus we conclude that the initialization cost in this case is $O(mn \log n)$ and the cost per iteration is $O(nm \log^2 m + mn \log n)$. We emphasize that if $m > n$, then one should consider using $\tilde{c}_F^{(1)}(A_{mn})$ as preconditioner instead.

§3.3 Separable Matrices.

Consider the following system $(A_m \otimes B_n)x = b$ where A_m is an m-by-m nonsingular matrix and B_n is an n-by-n Hermitian positive definite matrix. This system arises in solving the inverse heat problem in 2-D, see Chan [7]. Since $\delta^{(1)}(A_m \otimes B_n) = A_m \otimes \delta(B_n)$, it follows that

$$c_F^{(1)}(A_m \otimes B_n) = A_m \otimes c_F(B_n).$$

Thus the preconditioned system becomes

$$(A_m \otimes c_F(B_n))^{-1}(A_m \otimes B_n)x = (A_m \otimes c_F(B_n))^{-1}b,$$

or

$$(I \otimes c_F(B_n)^{-1}B_n)x = (A_m^{-1} \otimes c_F^{-1}(B_n))b.$$

For general B_n, $c_F(B_n)$ can be obtained in $O(n^2)$ operations and $c_F(B_n)^{-1}y$ can be obtained in $O(n \log n)$ operations for any vector y. By decomposing A_m into its LU factors first, we can then generate the new right hand side vector

$$(A_m^{-1} \otimes c_F^{-1}(B_n))b = (A_m^{-1} \otimes I)(I \otimes c_F^{-1}(B_n))b$$

in $O(m^3+m^2n+mn\log n+n^2)$ operations. In each subsequent iteration, the matrix-vector multiplication $(I \otimes c_F(B_n)^{-1}B_n)v$ can be done in $O(mn \log n + mn^2)$ operations.

When B_n is a Hermitian positive definite Toeplitz matrix, $c_F(B_n)$ can be obtained in $O(n)$ operation. Hence the initialization cost reduced to $O(m^3 + m^2n + mn\log n)$. Moreover, since the cost of multiplying $B_n y$ becomes $O(n \log n)$, we see that the cost per iteration decreases to $O(mn \log n)$.

§4 Convergence Rate.

In this section, we analyze the convergence rate of the preconditioned conjugate gradient method when applied to solving some special block systems.

§4.1 Quadrantally Symmetric Block Toeplitz Matrices.

Let us consider the system $T_{mn}x = b$ where T_{mn} is a quadrantally symmetric block Toeplitz matrix given by (20). Let the entries of the block $T_{(j)}$ be denoted by $t_{pq}^{(j)} = t_{|p-q|}^{(j)}$, for $1 \le p, q \le n, 0 \le j < m$. We assume that the generating sequence $t_k^{(j)}$ of T_{mn} is absolutely summable, i.e.

$$\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} |t_i^{(j)}| \le K < \infty \ .$$

In order to analyze the distribution of the eigenvalues of $T_{mn} - c_F^{(1)}(T_{mn})$, we need to introduce Strang's circulant preconditioner. For each $T_{(j)}$, Strang's preconditioner $s_F(T_{(j)})$ is defined to be the circulant matrix obtained by copying the central diagonals of $T_{(j)}$ and bringing them around to complete the circulant. More precisely, the entries $s_{pq}^{(j)} = s_{|p-q|}^{(j)}$ of $s_F(T_{(j)})$ are given by

$$s_k^{(j)} = \begin{cases} t_k^{(j)} & 0 \le k \le r, \\ t_{n-r}^{(j)} & r \le k < n. \end{cases} \tag{21}$$

Here for simplicity, we have assumed that $n = 2r$. Define

$$s_F^{(1)}(T_{mn}) = \begin{bmatrix} s_F(T_{(0)}) & s_F(T_{(1)}) & \cdots & s_F(T_{(m-1)}) \\ s_F(T_{(1)}) & s_F(T_{(0)}) & \cdots & s_F(T_{(m-2)}) \\ \vdots & \ddots & \ddots & \vdots \\ s_F(T_{(m-1)}) & s_F(T_{(m-2)}) & \cdots & s_F(T_{(0)}) \end{bmatrix} . \tag{22}$$

We prove below that the matrices $c_F^{(1)}(T_{mn})$ and $s_F^{(1)}(T_{mn})$ are asymptotically the same.

Lemma 5. *Let T_{mn} be given by (20) with an absolutely summable generating sequence. Then for all $m > 0$,*

$$\lim_{n\to\infty} \|s_F^{(1)}(T_{mn}) - c_F^{(1)}(T_{mn})\|_1 = 0 \ .$$

Proof. Let $B_{mn} \equiv s_F^{(1)}(T_{mn}) - c_F^{(1)}(T_{mn})$. By (17) and (22), we see that the block $B_{(j)}$ of B_{mn} are given by $s_F(T_{(j)}) - c_F(T_{(j)})$. Hence by (2) and (21) they are circulant with entries $b_{pq}^{(j)} = b_{|p-q|}^{(j)}$ given by

$$b_k^{(j)} = \begin{cases} \dfrac{k}{n}(t_k^{(j)} - t_{n-k}^{(j)}) & 0 \le k \le r, \\ \dfrac{n-k}{n}(t_{n-k}^{(j)} - t_k^{(j)}) & r \le k < n. \end{cases}$$

Thus

$$\|B_{mn}\|_1 \le 2\sum_{j=0}^{m-1} \|B_{(j)}\|_1 \le 2\sum_{j=0}^{m-1}\sum_{k=0}^{n-1} |b_k^{(j)}| \le 4\sum_{j=0}^{m-1}\sum_{k=1}^{r} \frac{k}{n}|t_k^{(j)}| + 4\sum_{j=0}^{m-1}\sum_{k=r+1}^{n-1} |t_k^{(j)}|.$$

For all $\varepsilon > 0$, since the generating sequence is absolutely summable, we can always find an $N_1 > 0$ and an $N_2 > 2N_1$, such that

$$\sum_{j=0}^{\infty}\sum_{k=N_1}^{\infty} |t_k^{(j)}| < \varepsilon \quad \text{and} \quad \frac{1}{N_2}\sum_{j=0}^{\infty}\sum_{k=1}^{N_1} k|t_k^{(j)}| < \varepsilon.$$

Thus for all $n > N_2$,

$$\|B_{mn}\|_1 \le \frac{4}{N_2}\sum_{j=0}^{\infty}\sum_{k=1}^{N_1} k|t_k^{(j)}| + 4\sum_{j=0}^{\infty}\sum_{k=N_1+1}^{r} |t_k^{(j)}| + 4\sum_{j=0}^{\infty}\sum_{k=r+1}^{\infty} |t_k^{(j)}| < 12\varepsilon \ . \qquad \square$$

In view of Lemma 5 and the following equality

$$T_{mn} - c_F^{(1)}(T_{mn}) = \left(s_F^{(1)}(T_{mn}) - c_F^{(1)}(T_{mn})\right) + \left(T_{mn} - s_F^{(1)}(T_{mn})\right) ,$$

we see that the spectra of $T_{mn} - c_F^{(1)}(T_{mn})$ and $T_{mn} - s_F^{(1)}(T_{mn})$ are asymptotically the same. However, it is easier to obtain spectral information about the second matrix as the following Lemma shows.

Lemma 6. *Let T_{mn} be given by (20) with an absolutely summable generating sequence. Then for all $\varepsilon > 0$, there exists an $N_3 > 0$, such that for all $n > N_3$ and for all $m > 0$,*

$$s_F^{(1)}(T_{mn}) - T_{mn} = W_{mn}^{(N_3)} + U_{mn}^{(N_3)},$$

where $\|W_{mn}^{(N_3)}\|_1 \le \varepsilon$ and rank$(U_{mn}^{(N_3)}) \le 2N_3 m$.

Proof. Define $W_{mn} \equiv s_F^{(1)}(T_{mn}) - T_{mn}$. It is clear from (21) that its blocks $W_{(j)} \equiv s_F(T_{(j)}) - T_{(j)}$ are symmetric Toeplitz matrices with entries $w_{pq}^{(j)} = w_{|p-q|}^{(j)}$ given by

$$w_k^{(j)} = \begin{cases} 0 & 0 \le k \le r \ , \\ t_{n-k}^{(j)} - t_k^{(j)} & r < k < n \ . \end{cases}$$

For all $\varepsilon > 0$, since the generating sequence is absolutely summable, there exists an $N_3 > 0$, such that $\sum_{j=0}^{\infty} \sum_{k=N_3}^{\infty} |t_k^{(j)}| < \varepsilon$. Corresponding to this N_3, we define, for each block $W_{(j)}$, the n-by-n matrix

$$W_{(j)}^{(N_3)} = \begin{bmatrix} \tilde{W}_{(j)} & 0 \\ 0 & 0 \end{bmatrix} ,$$

where $\tilde{W}_{(j)}$ is the $(n-N_3)$-by-$(n-N_3)$ principal submatrix of $W_{(j)}$. Clearly, each $\tilde{W}_{(j)}$ is a Toeplitz matrix. Let $U_{(j)}^{(N_3)} \equiv W_{(j)} - W_{(j)}^{(N_3)}$ for all j. We note that $U_{(j)}^{(N_3)}$ is nonzero only in the last N_3 rows and N_3 columns, therefore rank$(U_{(j)}^{(N_3)}) \le 2N_3$.

Let

$$W_{mn}^{(N_3)} = \begin{bmatrix} W_{(0)}^{(N_3)} & W_{(1)}^{(N_3)} & \cdots & W_{(m-1)}^{(N_3)} \\ W_{(1)}^{(N_3)} & W_{(0)}^{(N_3)} & \cdots & W_{(m-2)}^{(N_3)} \\ \vdots & \ddots & \ddots & \vdots \\ W_{(m-1)}^{(N_3)} & W_{(m-2)}^{(N_3)} & \cdots & W_{(0)}^{(N_3)} \end{bmatrix} , \qquad (23)$$

and

$$U_{mn}^{(N_3)} = \begin{bmatrix} U_{(0)}^{(N_3)} & U_{(1)}^{(N_3)} & \cdots & U_{(m-1)}^{(N_3)} \\ U_{(1)}^{(N_3)} & U_{(0)}^{(N_3)} & \cdots & U_{(m-2)}^{(N_3)} \\ \vdots & \ddots & \ddots & \vdots \\ U_{(m-1)}^{(N_3)} & U_{(m-2)}^{(N_3)} & \cdots & U_{(0)}^{(N_3)} \end{bmatrix} .$$

Then $s_F^{(1)}(T_{mn}) - T_{mn} = W_{mn}^{(N_3)} + U_{mn}^{(N_3)}$. Since each block $U_{(j)}^{(N_3)}$ in $U_{mn}^{(N_3)}$ is an n-by-n matrix where the leading $(n-N_3)$-by-$(n-N_3)$ principal submatrix is a zero matrix, it is easy to see that $\text{rank}(U_{mn}^{(N_3)}) \le 2N_3 m = O(m)$. For $W_{mn}^{(N_3)}$, we have by (23)

$$\begin{aligned} \|W_{mn}^{(N_3)}\|_1 &\le 2\sum_{j=0}^{m-1} \|W_{(j)}^{(N_3)}\|_1 = 2\sum_{j=0}^{m-1} \|\tilde{W}_{(j)}\|_1 \\ &= 2\sum_{j=0}^{m-1}\sum_{k=r+1}^{n-N_3-1} |w_k^{(j)}| = 2\sum_{j=0}^{m-1}\sum_{k=r+1}^{n-N_3-1} |t_{n-k}^{(j)} - t_k^{(j)}| \\ &\le 2\sum_{j=0}^{m-1}\sum_{k=N_3+1}^{n-N_3-1} |t_k^{(j)}| \le 2\sum_{j=0}^{\infty}\sum_{k=N_3}^{\infty} |t_k^{(j)}| < 2\varepsilon . \qquad \square \end{aligned}$$

Let $N = \max\{N_2, N_3\}$, where N_2 and N_3 are given in the proofs of Lemmas 5 and 6. Then for all $n > N$ and $m > 0$, we have

$$T_{mn} - c_F^{(1)}(T_{mn}) = M_{mn} + L_{O(m)} ,$$

where $M_{mn} = s_F^{(1)}(T_{mn}) - c_F^{(1)}(T_{mn}) + W_{mn}^{(N)}$ with $\|M_{mn}\|_1 < \varepsilon$ and $L_{O(m)} = U_{mn}^{(N)}$ with rank $(L_{O(m)}) = O(m)$. Since M_{mn} is symmetric, we have

$$\|M_{mn}\|_2 \le (\|M_{mn}\|_1 \|M_{mn}\|_\infty)^{\frac{1}{2}} = \|M_{mn}\|_1 < \varepsilon .$$

By using Cauchy's Interlace Theorem, we then have the following Theorem.

Theorem 4. *Let T_{mn} be given by (20) with an absolutely summable generating sequence. Then for all $\varepsilon > 0$, there exists an $N > 0$ such that for all $n > N$ and all $m > 0$, at most $O(m)$ eigenvalues of $c_F^{(1)}(T_{mn}) - T_{mn}$ have absolute values exceeding ε.*

If T_{mn} is positive definite with the smallest eigenvalue $\lambda_{\min}(T_{mn}) \ge \delta > 0$, where δ is independent of m and n, then by Theorem 1 (iv), $\lambda_{\min}\big(c_F^{(1)}(T_{mn})\big) \ge \delta > 0$. Hence $\|\big(c_F^{(1)}(T_{mn})\big)^{-1}\|_2$ is uniformly bounded. By noting that

$$\big(c_F^{(1)}(T_{mn})\big)^{-1} T_{mn} = I - \big(c_F^{(1)}(T_{mn})\big)^{-1}\big(c_F^{(1)}(T_{mn}) - T_{mn}\big),$$

we then have the following immediate Corollary.

Corollary 1. *Let T_{mn} be given by (20) with an absolutely summable generating sequence. If T_{mn} are positive definite for all m and n and that $\lambda_{\min}(T_{mn}) \geq \delta > 0$, then for all $\varepsilon > 0$, there exists an $N > 0$, such that for all $n > N$ and all $m > 0$, at most $O(m)$ eigenvalues of $\left(c_F^{(1)}(T_{mn})\right)^{-1} T_{mn} - I$ have absolute value large than ε.*

As a consequence, the spectrum of $\left(c_F^{(1)}(T_{mn})\right)^{-1} T_{mn}$ is clustered around 1 except for at most $O(m)$ outlying eigenvalues. When the preconditioned conjugate gradient method is applied to solving the system $T_{mn}x = b$, Corollary 1 shows that the number of iterations will grow at most like $O(m)$. We recall that in §3.2, the algorithm requires $O(mn \log n)$ operations in the initialization step and $O(mn \log^2 m + mn \log n)$ operations in each iteration. Thus the total complexity of the algorithm is bounded above by $O(m^2 n \log^2 m + m^2 n \log n)$.

We emphasize that for the quadrantally symmetric block Toeplitz systems we tested in §5, the number of iterations is independent of m and n and the complexity of the method is therefore of $O(nm \log^2 m + nm \log n)$.

We remark again that when $m > n$, one should consider using the preconditioner $\tilde{c}_F^{(1)}(T_{mn})$ instead. Then by repeating the whole argument we used, we can show that the preconditioned conjugate gradient method will converge in at most $O(n)$ steps for m sufficiently large. Hence the total complexity of the algorithm in this case is bounded above by $O(n^2 m \log^2 n + n^2 m \log m)$.

Before we close this subsection, we would like to point out that for quadrantally symmetric block Toeplitz matrix T_{mn}, we can define, analogous to $\tilde{c}_V^{(1)}(T_{mn})$, the matrix $\tilde{s}_F^{(1)}(T_{mn})$ as follows:

$$\tilde{s}_F^{(1)}(T_{mn}) = P^* s_F^{(1)}(P T_{mn} P^*) P,$$

where P is defined by (8). Then as in §2.3, we can further define the doubly circulant block preconditioner $\tilde{s}_F^{(1)} \circ s_F^{(1)}(T_{mn})$. As remarked after the proof of Theorem 3, $\tilde{s}_F^{(1)} \circ s_F^{(1)}(T_{mn})$ is the approximation of T_{mn} in two directions. Therefore it will not be a good preconditioner compared to either $s_F^{(1)}(T_{mn})$ or, in view of Lemma 5, to $c_F^{(1)}(T_{mn})$. We finally remark that if instead of Strang's circulant preconditioner, R. Chan's preconditioner [6] is used in (22), then the corresponding doubly circulant block preconditioner is the block preconditioner considered in Ku and Kuo [14].

§4.2 Separable Matrices.

Next we consider the system $(A_m \otimes T_n)x = b$ where T_n is a Toeplitz matrix with generating function f, i.e. the diagonals of T_n are given by the Fourier coefficients $a_j(f)$ of f. More precisely, we have

$$(T_n)_{jk} = a_{j-k}(f), \quad j,k = 1,2,\cdots .$$

We assume that f is positive, 2π-periodic and continuous and denote T_n by $T_n(f)$. For such $T_n(f)$, we have the following result, see Chan and Yeung [4].

Lemma 7. *Let f be a positive, 2π-periodic and continuous function. Then for all $\epsilon > 0$, there exist N and $M > 0$, such that for all $n > N$, at most M eigenvalues of the matrices $c_F^{-1}\big(T_n(f)\big)T_n(f) - I_n$ have absolute values large than ϵ.*

Since the preconditioned matrix is given by

$$\big[A_m \otimes c_F\big(T_n(f)\big)\big]^{-1}\big(A_m \otimes T_n(f)\big) = I_m \otimes \big[c_F^{-1}\big(T_n(f)\big)T_n(f)\big],$$

it is clear that the number of distinct eigenvalues of the preconditioned matrix is the same as the number of distinct eigenvalues of $c_F^{-1}\big(T_n(f)\big)T_n(f)$. In view of Lemma 7, we then see that for all $\epsilon > 0$, there exist N, $M > 0$, such that for all $n > N$ and all $m > 0$, at most M distinct eigenvalues of the matrices $\big\{I_m \otimes \big[c_F^{-1}\big(T_n(f)\big)T_n(f)\big]\big\} - I$ have absolute values large than ϵ. Thus the eigenvalues of the preconditioned matrix is clustered around 1 and hence the number of iterations required for convergence is a constant independent of n and m. Recalling the operation count in §3.3, the total complexity of the algorithm in this case is equal to $O(m^3 + nm^2 + mn\log n)$.

§5 Numerical Results.

In this section, we apply the preconditioned conjugate gradient method to the block systems we considered in §4. The stopping criteria for the method is set at $\frac{\|r_k\|_2}{\|r_0\|_2} < 10^{-7}$

where r_k is the residual vector at the kth iteration. The right hand side vector b is chosen to be the vector of all ones and the zero vector is the initial guess.

§5.1 Quadrantally Symmetric Block Toeplitz Matrices.

We consider T_{mn} of the form given in (20) with the diagonals of the blocks $T_{(j)}$ being given by $t_i^{(j)}$. Four different generating sequences were tested. They are

$$\text{(i)} \qquad t_i^{(j)} = \frac{1}{(j+1)(|i|+1)^{1+0.1\times(j+1)}}, \qquad j \geq 0,\ i = 0, \pm 1, \pm 2, \cdots,$$

$$\text{(ii)} \qquad t_i^{(j)} = \frac{1}{(j+1)^{1.1}(|i|+1)^{1+0.1\times(j+1)}}, \qquad j \geq 0,\ i = 0, \pm 1, \pm 2, \cdots,$$

$$\text{(iii)} \qquad t_i^{(j)} = \frac{1}{(j+1)^{1.1}+(|i|+1)^{1.1}}, \qquad j \geq 0,\ i = 0, \pm 1, \pm 2, \cdots,$$

$$\text{(iv)} \qquad t_i^{(j)} = \frac{1}{(j+1)^{2.1}+(|i|+1)^{2.1}}, \qquad j \geq 0,\ i = 0, \pm 1, \pm 2, \cdots.$$

The generating sequences (ii) and (iv) are absolutely summable while (i) and (iii) are not. Tables 1 and 2 show the number of iterations required for convergence. In all cases, we see that as $m = n$ increases, the number of iterations remains roughly a constant or increases very slowly for the preconditioned system with preconditioner $c_F^{(1)}(T_{mn})$ while it increases with other choices of preconditioners.

		Sequence (i)			Sequence (ii)		
$n = m$	mn	None	$c_F^{(1)}(T_{mn})$	$c_{F,F}^{(2)}(T_{mn})$	None	$c_F^{(1)}(T_{mn})$	$c_{F,F}^{(2)}(T_{mn})$
8	64	20	6	12	19	5	12
16	256	35	6	18	32	6	17
32	1024	43	6	21	41	6	20
64	4096	51	7	25	47	7	22
128	16384	54	7	26	50	7	24

Table 1. Preconditioners Used and the Number of Iterations

		Sequence (iii)			Sequence (iv)		
$n = m$	mn	None	$c_F^{(1)}(T_{mn})$	$c_{F,F}^{(2)}(T_{mn})$	None	$c_F^{(1)}(T_{mn})$	$c_{F,F}^{(2)}(T_{mn})$
8	64	18	7	16	14	7	12
16	256	40	8	30	22	8	20
32	1024	63	9	49	30	9	26
64	4096	101	11	80	36	9	33
128	16384	144	12	123	42	8	38

Table 2. Preconditioners Used and the Number of Iterations

§5.2 Separable Matrices.

We consider the separable block Toeplitz system $(\tilde{T}_m \otimes T_n)x = b$ where the diagonals of $\tilde{T}_m$ and T_n are given by $\tilde{t}_i = (|i|+1)^{-1}$ and $t_j = (|j|+1)^{-1.1}$ respectively for $i, j = 0, \pm 1, \pm 2, \cdots$. We note that $\tilde{T}_m \otimes T_n$ is also a quadrantally symmetric block Toeplitz matrix with the generating sequence given by

$$t_j^{(i)} = \frac{1}{(i+1)(|j|+1)^{1.1}}, \quad i \geq 0, \; j = 0, \pm 1, \pm 2, \cdots .$$

The preconditioner $c_F^{(1)}(\tilde{T}_m \otimes T_n)$ is given by $\tilde{T}_m \otimes c_F(T_n)$. Table 3 shows the number of iterations required for convergence. We notice that as $n = m$ increases, the number of iterations stays almost the same for the preconditioned system with preconditioner $c_F^{(1)}(\tilde{T}_m \otimes T_n)$ while it increases with other choices of preconditioners. We remark that since $\tilde{T}_m$ is a Toeplitz matrix, its inverse can be obtained in $O(m \log^2 m)$. Hence the total complexity of the algorithm is reduced to $O(mn \log^2 m + mn \log n)$.

$n = m$	mn	None	$c_F(\tilde{T}_m T_m) \otimes c_F(T_n)$	$\tilde{T}_m \otimes I_n$	$\tilde{T}_m \otimes c_F(T_n)$
8	64	20	7	5	4
16	256	34	9	10	4
32	1024	48	9	14	5
64	4096	57	10	18	5
128	16384	67	11	20	5

Table 3. Preconditioners Used and the Number of Iterations

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