Chapter 3

Iterative Methods for Linear Systems with Matrix Structure

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3.1. Introduction

Structured linear systems have been around for a long time and are encountered in various application fields. One interesting family consists of matrices having a Toeplitz form. An n-by-n matrix T_n is said to be *Toeplitz* if

$$T_n = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{2-n} & t_{1-n} \\ t_1 & t_0 & t_{-1} & & t_{2-n} \\ \vdots & t_1 & t_0 & \ddots & \vdots \\ t_{n-2} & & \ddots & \ddots & t_{-1} \\ t_{n-1} & t_{n-2} & \cdots & t_1 & t_0 \end{bmatrix}, \tag{3.1}$$

i.e., T_n is constant along its diagonals. Toeplitz systems arise in a variety of applications in mathematics and engineering, see Bunch [11] and the references therein. Since n-by-n Toeplitz matrices are determined by only $(2n-1)$ entries rather than n^2 entries, it is expected that the solution of Toeplitz systems can be obtained in less than $O(n^3)$ operations. In the literature, there are a number of fast direct Toeplitz solvers and superfast direct Toeplitz solvers with complexity $O(n^2)$ and $O(n \log^2 n)$ operations respectively, see [11, 60] and the references therein.

Another interesting family consists of matrices having a Hankel form. An n-by-n matrix H_n is said to be *Hankel* if

$$H_n = \begin{bmatrix} h_0 & h_1 & \cdots & h_{n-2} & h_{n-1} \\ h_1 & h_2 & \iddots & \iddots & h_n \\ \vdots & \iddots & \iddots & \iddots & \vdots \\ h_{n-2} & \iddots & \iddots & \iddots & h_{2n-2} \\ h_{n-1} & h_n & \cdots & h_{2n-2} & h_{2n-1} \end{bmatrix}, \tag{3.2}$$

[0] This chapter will appear in *Fast Reliable Algorithms for Matrices with Structure*, ed: T. Kailath and A. Sayed, SIAM.

i.e., H_n is constant along its antidiagonals.

In signal processing, solutions of Toeplitz-like or Toeplitz-plus-Hankel systems are required in order to obtain the filter coefficients in the design of the digital filters, see Haykin [55]. By using Goursat functions and conformal mapping methods, the numerical solutions of biharmonic equations can be obtained by solving a system where the coefficient matrix is the sum of the identity matrix and a Hankel matrix, see Muskhelishvili [71]. In image processing, deconvolution problems involve solutions of Toeplitz-plus-band systems for the unknown image [87, 17]. These applications have motivated both mathematicians and engineers to develop specific algorithms catering to solving these linear systems with matrix structure.

In this chapter, we survey some of the latest developments on using preconditioned conjugate gradient (PCG) methods for solving n-by-n linear systems with matrix structure. Here the coefficient matrices are Toeplitz, Toeplitz-like, Toeplitz-plus-Hankel or Toeplitz-plus-band. The motivation for using iterative methods for solving linear systems with matrix structure is that the matrix-vector products $A_n y$ where A_n are Toeplitz, Toeplitz-like, Toeplitz-plus-Hankel or Toeplitz-plus-band, can be computed efficiently. For instance, for n-by-n Toeplitz-like or Toeplitz-plus-Hankel matrices, their matrix-vector multiplications can be computed in $O(n \log n)$ operations using Fast Fourier Transform (FFT); for Toeplitz-plus-band matrix where the band matrix has bandwidths ν, its matrix-vector product can be calculated in $O(n \log n + \nu n)$ operations. Thus the solutions of these structured linear systems can be obtained in $O(n \log n)$ operations with the proper choice of preconditioner for these structured coefficient matrices. Moreover, the basic tool of the PCG algorithm is the FFT which is highly parallelizable and has been implemented on multiprocessors efficiently [2, p.238] and [80]. Since conjugate gradient methods are easily parallelizable too [6, p.165], the preconditioned conjugate gradient method is well-adapted for parallel computing. Besides the reduction of the arithmetic complexity, there are some structured linear systems where the direct solvers are notoriously unstable, e.g., indefinite and certain non-Hermitian Toeplitz-plus-Hankel matrices. Therefore, iterative methods provide alternatives to solving these systems.

The outline of this chapter is as follows. In the next two sections, we recall some results of using the preconditioned conjugate gradient method for solving Toeplitz systems. Applications of PCG methods for linear systems with matrix structure are discussed. Some useful and successful preconditioners for these structured coefficient matrices are also considered. Finally, some concluding remarks are given.

3.2. Iterative Methods for Solving Toeplitz Systems

Recent research on using the preconditioned conjugate gradient (PCG) method as an iterative method for solving Toeplitz systems has brought much attention, see the survey paper by Chan and Ng [29]. In the following, we recall some of the results in solving Toeplitz systems by the preconditioned conjugate gradient method.

Let us begin by introducing the notation that will be used throughout the chapter. Let $\mathbf{C}_{2\pi}$ be the set of all 2π-periodic continuous complex-valued functions defined on $[-\pi, \pi]$. For all $f \in \mathbf{C}_{2\pi}$, let

$$t_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)e^{-ik\theta}d\theta, \quad k = 0, \pm 1, \pm 2, \cdots$$

be the Fourier coefficients of f. For all $n \geq 1$, let T_n be the n-by-n Toeplitz matrix with entries $t_{j,k} = t_{j-k}$, $0 \leq j, k < n$. The function f is called the *generating function* of the sequence of Toeplitz matrices T_n, see Grenander and Szegö [52]. If f is a real-valued function, we have

$$t_{-k} = \bar{t}_k, \quad k = 0, \pm 1, \pm 2, \cdots.$$

It follows that T_n are Hermitian matrices. Note that when f is an even real-valued function, the matrices T_n are real symmetric.

We emphasize that in practical applications, the functions f are readily available. Typical examples of generating functions are the kernels of Wiener-Hopf equations, see Gohberg and Fel'dman [49, p.82], the functions which give the amplitude characteristics of recursive digital filters, see Chui and A. Chan [39], the spectral density functions in stationary stochastic processes, see Grenander and Szegö [52, p.171], and the point-spread functions in image deblurring, see Jain [59, p.269].

We will solve the systems $A_n x = b$ by conjugate gradient methods. The convergence rate of the methods depends partly on how clustered the spectra of the sequence of matrices A_n are, see Axelsson and Barker [3, p.24]. The clustering of the spectra of a sequence of matrices is defined as follows:

DEFINITION 3.2.1. *A sequence of matrices $\{A_n\}_{n=1}^{\infty}$ is said to have clustered spectra around 1 if for any given $\epsilon > 0$, there exist positive integers n_1 and n_2 such that for all $n > n_1$, at most n_2 eigenvalues of the matrix $A_n - I_n$ have absolute value larger than ϵ.*

For Toeplitz matrices, we note that there is a close relationship between the spectrum of T_n and its generating function f.

THEOREM 3.2.1. **(Grenander and Szegö Grenander)** *Let f be a 2π-periodic continuous real-valued function. Then the spectrum $\lambda(T_n)$ of T_n satisfies*

$$\lambda(T_n) \subseteq [f_{\min}, f_{\max}], \quad \forall n \geq 1, \tag{3.3}$$

where $f_{\min}$ and $f_{\max}$ are the minimum and maximum values of f, respectively. Moreover, the eigenvalues $\lambda_j(T_n)$, $j = 0, 1, \ldots, n-1$, are equally distributed as $f(2\pi j/n)$, i.e.,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1}\left[g(\lambda_j(T_n)) - g(f(\frac{2\pi j}{n}))\right] = 0 \tag{3.4}$$

for any continuous function g defined on $[-\pi, \pi]$.

The equal distribution of eigenvalues of Toeplitz matrices indicates that the eigenvalues will not be clustered in general. One way to speed up the convergence rate of the method is to precondition the Toeplitz system. Thus, instead of solving $T_n x = b$, we solve the preconditioned system

$$P_n^{-1} T_n x = P_n^{-1} b. \tag{3.5}$$

The preconditioner P_n should be chosen according to the following criteria:

- P_n should be constructed within $O(n \log n)$ operations.
- $P_n v = y$ should be solved in $O(n \log n)$ operations.
- The spectrum of $P_n^{-1} T_n$ should be clustered and/or the condition number of the preconditioned matrix should be close to 1.

In the next three subsections, we will review three different kinds of preconditioners developed for Toeplitz systems that satisfy the three criteria mentioned above.

3.2.1. Circulant Preconditioners In 1986, Strang [79] and Olkin [75] independently proposed the use of circulant matrices to precondition Toeplitz matrices in conjugate gradient iterations. Part of their motivation is to exploit the fast inversion of circulant matrices.

An n-by-n matrix C_n is said to be *circulant* if

$$C_n = \begin{bmatrix} c_0 & c_{-1} & \cdots & c_{2-n} & c_{1-n} \\ c_1 & c_0 & c_{-1} & & c_{2-n} \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & & \ddots & \ddots & c_{-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{bmatrix},$$

where $c_{-k} = c_{n-k}$ for $1 \le k \le n-1$. Circulant matrices are diagonalized by the Fourier matrix F_n, i.e.,

$$C_n = F_n^* \Lambda_n F_n \tag{3.6}$$

where the entries of F_n are given by

$$[F_n]_{j,k} = \frac{1}{\sqrt{n}} e^{2\pi ijk/n}, \quad 0 \le j, k \le n-1,$$

and Λ_n is a diagonal matrix holding the eigenvalues of C_n, see for instance Davis [46, p.73].

We note that Λ_n can be obtained in $O(n \log n)$ operations by taking the fast Fourier transform (FFT) of the first column of C_n. For the fast Fourier transform algorithm, we refer to Cooley and Tukey [43]. In fact, the diagonal entries λ_k of Λ_n are given by

$$\lambda_k = \sum_{j=0}^{n-1} c_j e^{2\pi ijk/n}, \quad k = 0, \ldots, n-1. \tag{3.7}$$

Once Λ_n is obtained, the products $C_n y$ and $C_n^{-1} y$ for any vector y can be computed by FFTs in $O(n \log n)$ operations using (3.6).

With circulant matrices as preconditioners, in each iteration, we have to solve a circulant system. From (3.6), we see that circulant matrices can be diagonalized by discrete Fourier matrices, and hence the inversion of n-by-n circulant systems can be done in $O(n \log n)$ operations by using FFTs of size n. The matrix-vector multiplications $T_n y$ can also be computed by FFTs by first embedding A into a $2n$-by-$2n$ circulant matrix, i.e.,

$$\begin{bmatrix} T_n & \times \\ \times & T_n \end{bmatrix} \begin{bmatrix} y \\ 0 \end{bmatrix} = \begin{bmatrix} T_n y \\ \dagger \end{bmatrix},$$

see [29], and then carrying out the multiplication by using the decomposition of circulant matrices. The matrix-vector multiplication thus requires $O(2n \log(2n))$ operations. It follows that the total number of operations per iteration is of $O(n \log n)$ operations.

Strang's Preconditioner Several successful circulant preconditioners have been proposed and analyzed, see [29]. One of the successful circulant preconditioners is Strang's circulant preconditioner. For an n-by-n Toeplitz matrix T_n, Strang's circulant preconditioner [79] is defined to be the matrix that copies the central diagonals of T_n and reflects them around to complete the circulant requirement. For T_n given by (3.1), the diagonals s_j of the Strang preconditioner $S_n = [s_{k-\ell}]_{0 \le k, \ell < n}$ are given by

$$s_j = \begin{cases} t_j, & 0 < j \le \lfloor n/2 \rfloor, \\ t_{j-n} & \lfloor n/2 \rfloor < j < n, \\ s_{n+j}, & 0 < -j < n. \end{cases} \tag{3.8}$$

The approach developed in the following convergence proof (Theorems 3.2.2 and 3.2.3 and Corollary 3.2.1) of Strang's preconditioned system have been adapted by other authors to establish the convergence proof of other circulant preconditioned systems. The main idea of the proof is to show that the preconditioned matrices $S_n^{-1} T_n$ can be written as the form $I_n + L_n + U_n$ where I_n is an n-by-n identity matrix, L_n is a matrix of low rank and U_n is a matrix of small ℓ_2-norm. It follows that the preconditioned conjugate gradient methods, when applied to the preconditioned system, converges superlinearly.

The first step of the proof on the clustered spectra of $S_n^{-1} T_n$ is to show that S_n and S_n^{-1} are uniformly bounded in ℓ_2-norm.

THEOREM 3.2.2. **(R. Chan [13])** *Let f be a positive real-valued function in the Wiener class, i.e., its Fourier coefficients are absolutely summable,*

$$\sum_{k=0}^{\infty} |t_k| < \infty.$$

Then for large n, the circulants S_n and S_n^{-1} are uniformly bounded in ℓ_2-norm.

Proof. By (3.7), the jth eigenvalue of S_n is equal to

$$\sum_{k=1-m}^{m} t_k e^{2\pi ijk/n}.$$

Since the infinite series $\sum_{-\infty}^{\infty} t_k e^{ik\theta}$ is absolutely convergent and its sum f satisfies $f \geq \delta > 0$, the partial sums are uniformly positive for large n. The result follows. $\square$

THEOREM 3.2.3. **(R. Chan [13])** *Let f be a real-valued function in the Wiener class. Let $\{T_n\}$ be the sequence of Toeplitz matrices generated by f. Then the spectra of $S_n - T_n$ are clustered around zero for large n.*

Proof. For simplicity, we are assuming here and in the following that $n = 2m+1$. The case where $n = 2m$ can be treated similarly.

Clearly $B_n = S_n - T_n$ is a Hermitian Toeplitz matrix with entries $b_{ij} = b_{i-j}$ given by

$$b_k = \begin{cases} 0 & 0 \leq k \leq m, \\ t_{k-n} - t_k & m < k < n, \\ \bar{b}_{-k} & 0 < -k < n. \end{cases} \tag{3.9}$$

Since f is in the Wiener class, for all given $\epsilon > 0$, there exists an $N > 0$, such that $\sum_{k=N+1}^{\infty} |t_k| < \epsilon$. Let $U_n^{(N)}$ be the n by n matrix obtained from B_n by replacing the $(n-N)$ by $(n-N)$ leading principal submatrix of B_n by the zero matrix. Then $\operatorname{rank}(U_n^{(N)}) \leq 2N$.

Let $W_n^{(N)} \equiv B_n - U_n^{(N)}$. The leading $(n-N)$ by $(n-N)$ block of $W_n^{(N)}$ is the leading $(n-N)$ by $(n-N)$ principal submatrix of B_n, hence this block is a Toeplitz matrix, and it is easy to see that the maximum absolute column sum of $W_n^{(N)}$ is attained at the first column (or the $(n-N-1)$-th column). Thus

$$||W_n^{(N)}||_1 = \sum_{k=m+1}^{n-N-1} |b_k| = \sum_{k=m+1}^{n-N-1} |t_{k-n} - t_k| \leq \sum_{k=N+1}^{n-N-1} |t_k| < \epsilon.$$

Since $W_n^{(N)}$ is Hermitian, we have $||W_n^{(N)}||_\infty = ||W_n^{(N)}||_1$. Thus

$$||W_n^{(N)}||_2 \leq (||W_n^{(N)}||_1 \cdot ||W_n^{(N)}||_\infty)^{\frac{1}{2}} < \epsilon.$$

Hence the spectrum of $W_n^{(N)}$ lies in $(-\epsilon, \epsilon)$. By Cauchy Interlace Theorem, see Wilkinson [88], we see that at most $2N$ eigenvalues of $B_n = S_n - T_n$ have absolute values exceeding ϵ. $\square$

Using the fact that $S_n^{-1}T_n$ is similar to $S_n^{-1/2}T_nS_n^{-1/2}$, the result of Theorem 3.2.2 and

$$S_n^{-1/2}T_nS_n^{-1/2} = I_n + S_n^{-1/2}(T_n - S_n)S_n^{-1/2},$$

we can conclude that the spectra of $S_n^{-1}T_n$ are clustered around 1 for large n.

It follows easily from Theorems 3.2.2 and 3.2.3 that the conjugate gradient method, when applied to solving the preconditioned system

$$S_n^{-1}T_n x = S_n^{-1}b,$$

converges superlinearly for large n, see [32].

COROLLARY 3.2.1. *Let f be a positive real-valued function in the Wiener class. Let $\{T_n\}$ be the sequence of Toeplitz matrices generated by f. Then for any given $\epsilon > 0$, there exists a constant $c(\epsilon) > 0$ such that the error vector e_k of the preconditioned conjugate gradient method at the kth iteration satisfies*

$$\frac{|||e_k|||}{|||e_0|||} \le c(\epsilon)\epsilon^k \tag{3.10}$$

where

$$|||v|||^2 \equiv v^* S_n^{-1/2} T_n S_n^{-1/2} v.$$

If extra smoothness conditions are imposed on the generating function f (or on the sequence $\{t_k\}$), we can get more precise estimates on how $|||e_q|||$ in (3.10) goes to zero.

THEOREM 3.2.4. **(R. Chan [13])** *Let f be an $(\ell+1)$-times differentiable real-valued function with $f^{(\ell+1)} \in L^1[-\pi,\pi]$ where $\ell > 0$ (i.e. $|t_j| \le \hat{c}/j^{\ell+1}$ for some constant $\hat{c}$.) Then there exists a constant c which depends only on f and ν, such that for large n,*

$$\frac{|||e_{2q}|||}{|||e_0|||} \le \frac{c^q}{((q-1)!)^{2\ell}}. \tag{3.11}$$

Proof. We remark that from the standard error analysis of the conjugate gradient method, we have

$$|||e_k||| \le [\, \min_{P_k} \max_{\lambda} |P_k(\lambda)|\,]\; |||e_0||| \tag{3.12}$$

where the minimum is taken over polynomials of degree k with constant term 1 and the maximum is taken over the spectrum of $S_n^{-1/2}T_nS_n^{-1/2}$.

In the following, we will try to estimate that minimum in (3.12). We first note that the assumptions on f imply that

$$|t_j| \le \frac{\hat{c}}{|j|^{l+1}}, \quad \forall j,$$

where $\hat{c} = ||f^{(l+1)}||_{L^1}$, see, for instance, Katznelson [62]. Hence

$$\sum_{j=k+1}^{n-k-1} |t_j| \le \hat{c} \sum_{j=k+1}^{n-k-1} \frac{1}{|j|^{l+1}} \le \hat{c}\int_k^{\infty} \frac{dx}{x^{l+1}} \le \frac{\hat{c}}{k^l}, \quad \forall k \ge 1.$$

As in Theorem 3.2.3, we write

$$B_n = W_n^{(k)} + U_n^{(k)}, \quad \forall k \ge 1,$$

where $U_n^{(k)}$ is the matrix obtained from B_n by replacing its $(n-k)$ by $(n-k)$ principal submatrix of B_n by a zero matrix. Using the arguments in Theorem 3.2.3, we see that $\mathrm{rank}(U_n^{(k)}) \le 2k$ and $||W_n^{(k)}||_2 \le \hat{c}/k^l$, for all $k \ge 1$. Now consider

$$S_n^{-\frac{1}{2}} B_n S_n^{-\frac{1}{2}} = S_n^{-\frac{1}{2}} W_n^{(k)} S_n^{-\frac{1}{2}} + S_n^{-\frac{1}{2}} U_n^{(k)} S_n^{-\frac{1}{2}} \equiv \tilde{W}_n^{(k)} + \tilde{U}_n^{(k)}.$$

By Theorem 3.2.3, we have, for large n, $\mathrm{rank}(\tilde{U}_n^{(k)}) \le 2k$ and

$$||\tilde{W}_n^{(k)}||_2 \le ||S_n^{-1}||_2 ||W_n^{(k)}||_2 \le \frac{\tilde{c}}{k^l}, \quad \forall k \ge 1,$$

with $\tilde{c} = \hat{c}/f_{\min}$.

Next we note that $W_n^{(k)} - W_n^{(k+1)}$ can be written as the sum of two rank one matrices of the form:

$$W_n^{(k)} - W_n^{(k+1)} = u_k v_k^* + v_k u_k^* = \frac{1}{2}(w_k^+ w_k^{+*} - w_k^- w_k^{-*}), \quad \forall k \ge 0.$$

Here u_k is the $(n-k)$-th unit vector,

$$v_k = [b_{n-k-1}, \cdots, b_1, b_0/2, 0, \cdots, 0]^T$$

with b_j given by (3.9), and $w_k^{\pm} = u_k \pm v_k$. Hence by letting $z_k^{\pm} = S_n^{-\frac{1}{2}} w_k^{\pm}$ for $k \ge 0$, we have

$$\begin{aligned} S_n^{-\frac{1}{2}} B_n S_n^{-\frac{1}{2}} &= \tilde{W}_n^{(0)} = \tilde{W}_n^{(k)} + \frac{1}{2}\sum_{j=0}^{k-1}(z_j^+ z_j^{+*} - z_j^- z_j^{-*}), \\ &= \tilde{W}_n^{(k)} + V_k^+ - V_k^-, \quad \forall k \ge 1, \end{aligned} \tag{3.13}$$

where $V_k^{\pm} \equiv \frac{1}{2}\sum_{j=0}^{k-1} z_j^{\pm} z_j^{\pm *}$ are positive semi-definite matrices of rank k.

Let us order the eigenvalues of $\tilde{W}_n^{(0)}$ as

$$\mu_0^- \le \mu_1^- \le \cdots \le \mu_1^+ \le \mu_0^+.$$

By applying Cauchy Interlace Theorem to and using the bound of $||\tilde{W}_n^{(k)}||_2$ in (3.13), we see that for all $k \ge 1$, there are at most k eigenvalues of $\tilde{W}_n^{(0)}$ lying to the right of $\tilde{c}/k^l$, and there are at most k of them lying to the left of $-\tilde{c}/k^l$. More precisely, we have

$$|\mu_k^{\pm}| \le ||\tilde{W}_n^{(k)}||_2 \le \frac{\tilde{c}}{k^l}, \quad \forall k \ge 1.$$

Using the identity

$$S_n^{-\frac{1}{2}} A_n S_n^{-\frac{1}{2}} = I_n + S_n^{-\frac{1}{2}} B_n S_n^{-\frac{1}{2}} = I_n + \tilde{W}_n^{(0)},$$

we see that if we order the eigenvalues of $S_n^{-\frac{1}{2}} A_n S_n^{-\frac{1}{2}}$ as

$$\lambda_0^- \le \lambda_1^- \le \cdots \le \lambda_1^+ \le \lambda_0^+, \tag{3.14}$$

then $\lambda_k^\pm = 1 + \mu_k^\pm$ for all $k \ge 0$ with

$$1 - \frac{\tilde{c}}{k^l} \le \lambda_k^- \le \lambda_k^+ \le 1 + \frac{\tilde{c}}{k^l}, \quad \forall k \ge 1. \tag{3.15}$$

For $\lambda_0^\pm$, the bounds are obtained from Theorem 3.2.1:

$$\frac{f_{\min}}{f_{\max}} \le \lambda_0^- \le \lambda_0^+ \le \frac{f_{\max}}{f_{\min}}. \tag{3.16}$$

Having obtained the bounds for $\lambda_k^\pm$, we can now construct the polynomial that will give us a bound for (3.12). Our idea is to choose P_{2q} that annihilates the q extreme pairs of eigenvalues. Thus consider

$$p_k(x) = (1 - \frac{x}{\lambda_k^+})(1 - \frac{x}{\lambda_k^-}), \quad \forall k \ge 1.$$

Between those roots $\lambda_k^\pm$, the maximum of $|p_k(x)|$ is attained at the average $x = \frac{1}{2}(\lambda_k^+ + \lambda_k^-)$, where by (3.14), (3.15) and (3.16), we have

$$\max_{x \in [\lambda_k^-, \lambda_k^+]} |p_k(x)| = \frac{(\lambda_k^+ - \lambda_k^-)^2}{4\lambda_k^+ \lambda_k^-} \le (\frac{2\tilde{c}}{k^l})^2 \cdot (\frac{f_{\max}}{2f_{\min}})^2 = (\frac{\tilde{c} f_{\max}}{f_{\min}})^2 \cdot \frac{1}{k^{2l}}, \quad \forall k \ge 1,$$

Similarly, for $k = 0$, we have, by using (3.16),

$$\max_{x \in [\lambda_0^-, \lambda_0^+]} |p_0(x)| = \frac{(\lambda_0^+ - \lambda_0^-)^2}{4\lambda_0^+ \lambda_0^-} \le \frac{(f_{\max}^2 - f_{\min}^2)^2}{4 f_{\min}^4}.$$

Hence the polynomial $P_{2q} = p_0 p_1 \cdots p_{q-1}$, which annihilates the q extreme pairs of eigenvalues, satisfies

$$|P_{2q}(x)| \le \frac{c^q}{((q-1)!)^{2l}}, \tag{3.17}$$

for some constant c that depends only on f and l. This holds for all $\lambda_k^\pm$ in the inner interval between λ_{q-1}^- and λ_{q-1}^+, where the remaining eigenvalues are. Equation (3.11) now follows directly from (3.12) and (3.17). $\square$

Other precise estimates on how $|||e_q|||$ in (3.10) goes to zero under different smoothness conditions can be found in [83, 65, 66, 34].

T. Chan's Preconditioner For an n-by-n Toeplitz matrix T_n, T. Chan's circulant preconditioner $c(T_n)$ is defined to be the minimizer of

$$||C_n - T_n||_F \tag{3.18}$$

over all n-by-n circulant matrices C_n, see T. Chan [36]. Here $\|\cdot\|_F$ denotes the Frobenius norm. In [36], the matrix $c(T_n)$ is called an *optimal* circulant preconditioner because it minimizes (3.18). The jth diagonals of $c(T_n)$ are shown to be equal to

$$c_j = \begin{cases} \dfrac{(n-j)t_j + jt_{j-n}}{n}, & 0 \le j < n, \\ c_{n+j}, & 0 < -j < n, \end{cases} \tag{3.19}$$

which are just the average of the diagonals of T_n, with the diagonals being extended to length n by a wrap-around.

By using (3.7) and (3.19), we see that the eigenvalues $\lambda_k(c(T_n))$ of $c(T_n)$ are given by

$$\lambda_k(c(T_n)) = \sum_{j=-n+1}^{n-1} t_j \left(1 - \frac{|j|}{n}\right) e^{2\pi ijk/n}, \quad k = 0, \ldots, n-1. \tag{3.20}$$

For the performance of $c(T_n)$ as preconditioners for Toeplitz matrices T_n, R. Chan [14] has proved that under the Wiener class assumptions in Theorem 3.2.3 (i.e., f is a positive function with absolutely summable Fourier coefficients), the spectra of $c(T_n) - T_n$ and $S_n - T_n$ are asymptotically the same as n tends to infinity, i.e., $\lim_{n\to\infty} ||c(T_n) - S_n||_2 = 0$. Hence, $c(T_n)$ works as well for Wiener class functions as S_n does.

THEOREM 3.2.5. **(R. Chan [14])** *Let f be a real-valued function in the Wiener class. Let $\{T_n\}$ be the sequence of Toeplitz matrices generated by f. Then*

$$\lim_{n\to\infty} \rho\left(S_n - c(T_n)\right) = 0,$$

where $\rho(\cdot)$ denotes the spectral radius.

Proof. By (3.8) and (3.19), it is clear that $B_n \equiv S_n - c(T_n)$ is circulant with entries

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

Here for simplicity, we are still assuming $n = 2m$. Using the fact that the j-th eigenvalue $\lambda_j(B_n)$ of B_n is given by $\sum_{k=0}^{n-1} b_k e^{2\pi ijk/n}$, we have

$$\lambda_j(B_n) = 2\sum_{k=1}^{m-1} \frac{k}{n}(t_k - t_{n-k})\cos(2\pi jk/n).$$

This implies

$$\rho(B_n) \le 2\sum_{k=1}^{m-1} \frac{k}{n}|t_k| \;+\; 2\sum_{k=m+1}^{n-1} |t_k|.$$

Since f is in the Wiener class, hence for all $\epsilon > 0$, we can always find an $M_1 > 0$ and an $M_2 > M_1$, such that

$$\sum_{k=M_1+1}^{\infty} |t_k| < \epsilon/6 \quad \text{and} \quad \frac{1}{M_2}\sum_{k=1}^{M_1} k|t_k| < \epsilon/6.$$

Thus for all $m > M_2$,

$$\rho(B_n) < \frac{2}{M_2}\sum_{k=1}^{M_1} k|t_k| + 2\sum_{k=M_1+1}^{m-1} |t_k| + 2\sum_{k=m+1}^{\infty} |t_k| < \epsilon. \quad \square$$

For an n-by-n general non-Toeplitz matrix A_n, the circulant minimizer $c(A_n)$ of $\|C_n - A_n\|_F$ can still be defined and obtained easily by taking the arithmetic average of the entries of A_n, i.e., its diagonals are given by

$$c_\ell = \frac{1}{n}\sum_{j-k=\ell (\mathrm{mod}\ n)} a_{j,k}, \quad \ell = 0, \ldots, n-1, \tag{3.21}$$

see [84]. Therefore, T. Chan's preconditioner is particularly useful in solving non-Toeplitz systems arising from the numerical solutions of elliptic partial differential equations [16] and Toeplitz least squares problems arising from signal and image processing [24, 25, 26, 37, 74]. Convergence results for T. Chan's preconditioner have been established for these problems, see [29]. One good property of the T. Chan preconditioner is that it preserves the positive-definiteness of a given matrix.

THEOREM 3.2.6. **(Tyrtyshnikov [84], R. Chan, X. Jin and M. Yeung [22])** *If A_n is Hermitian positive definite, then $c(A_n)$ is Hermitian and positive definite. Moreover, we have*

$$\lambda_{\min}(A_n) \le \lambda_{\min}(c(A_n)) \le \lambda_{\max}(c(A_n)) \le \lambda_{\max}(A_n). \tag{3.22}$$

Proof. Tyrtyshnikov [84] first proved it for the real scalar field and R. Chan, Jin, and Yeung [22] generalized the result to the complex field. By (3.21), it is clear that $c(A_n)$ is Hermitian when A_n is Hermitian. As the Frobenius norm is a unitary-invariant norm, the minimizer of $||C_n - A_n||_F$ over all C_n of the form $C = F^*\Lambda F$, Λ a diagonal matrix, is attained at $F_n\Delta_n F_n^*$. Here Δ_n is a diagonal matrix with diagonal entries

$$[\Delta_n]_{j,j} = [F_n A_n F_n^*]_{j,j} \equiv \lambda_j, \quad j = 1, \ldots, n.$$

Suppose that $\lambda_j = \lambda_{\min}(c(A_n))$ and $\lambda_k = \lambda_{\max}(c(A_n))$. Let e_j and e_k denote the j-th and the k-th unit vectors respectively. Since A_n is Hermitian, we have

$$\begin{aligned} \lambda_{\max}(c(A_n)) &= \lambda_k = \frac{e_k^* F_n A_n F_n^* e_k}{e_k^* e_k} \le \max_{x\neq 0} \frac{x^* F_n A_n F_n^* x}{x^* x} \\ &= \max_{x \neq 0} \frac{x^* A_n x}{x^* x} = \lambda_{\max}(A_n). \end{aligned}$$

Similarly,

$$\begin{aligned}\lambda_{\min}(A_n) &= \min_{x\neq 0}\frac{x^*A_nx}{x^*x} = \min_{x\neq 0}\frac{x^*F_nA_nF_n^*x}{x^*x} \le \frac{e_j^*F_nA_nF_n^*e_j}{e_j^*e_j}\\ &= \lambda_j = \lambda_{\min}(c(A_n)).\end{aligned}$$

From the inequality above, we can easily see that $c(A_n)$ is positive definite when A_n is positive definite. □

Besides Strang's and T. Chan's circulant preconditioners, R. Chan [13] and Ku and Kuo [63] have also constructed circulant preconditioners by embedding. Instead of using the minimizer of $\|C_n - T_n\|_F$ as preconditioners, Huckle [57], Tyrtyshnikov [84] and Tismenetsky [81] have considered circulant preconditioners that are minimizers of other approximations. As alternatives to circulant preconditioners, Toeplitz matrices [28, 54] and other transformed based preconditioners [9, 31, 7, 8, 61] have also been proposed and analyzed as preconditioners for Toeplitz systems. For details, see our recent survey paper [29].

3.2.2. Band-Toeplitz Preconditioners In this subsection, we consider Toeplitz matrices T_n generated by non-negative 2π-periodic real-valued functions. We first recall that a function f is said to have a νth order zero at θ_0 if $f(\theta_0) = 0$ and ν is the smallest positive integer such that $f^{(\nu)}(\theta_0) \neq 0$ and $f^{(\nu+1)}(\theta)$ is continuous in a neighborhood of θ_0. With the knowledge of the order of f at its minimum, we can give a better estimate of the spectrum of T_n than that in (3.3).

THEOREM 3.2.7. **(R. Chan [15])** *Suppose that $f(\theta) - f_{\min}$ has a unique zero of order 2ν at $\theta = \theta_0$. Let $\{T_n\}$ be the sequence of Toeplitz matrices generated by f. Then for all $n > 0$, we have*

$$\lambda_{\min}(T_n) \le d_1 f_{\min} + d_2 n^{-2\nu},$$

and the condition number $\kappa(T_n)$ of T_n satisfies

$$\kappa(T_n) \ge \frac{d_3 n^{2\nu}}{d_4 + f_{\min} n^{2\nu}},$$

where $\{d_i\}_{i=1}^4$ are some constants independent of n.

Thus when $f_{\min} = 0$, the condition number of T_n is not uniformly bounded and the Toeplitz matrix T_n is ill-conditioned. Tyrtyshnikov has proved theoretically [85] that Strang's preconditioner will fail in this case. In fact, he showed that if f is such that its μth derivative $f^{(\mu)}$ is piecewise continuous and has a bounded derivative on each continuity interval, the number of outlying eigenvalues of $S_n^{-1}T_n$ is of $O(n^{\nu/(\nu+\mu)})$. Here ν is the order of f at the zeros.

Instead of finding other possible circulant preconditioners, R. Chan [15] resorted to using band-Toeplitz matrices as preconditioners. The motivation behind using band-Toeplitz matrices is to approximate the generating function

f by trigonometric polynomials of fixed degree rather than by convolution products of f with some kernels. The advantage here is that trigonometric polynomials can be chosen to match the zeros of f, so that the preconditioned method still works when f has zeros.

THEOREM 3.2.8. **(R. Chan [15] and R. Chan and M. Ng [27])** *Let f be a non-negative piecewise continuous real-valued function defined on $[-\pi, \pi]$. Suppose that $f(\theta) - f_{\min}$ has a unique zero of order 2ν at $\theta = \theta_0$. Let $\{T_n\}$ be the sequence of Toeplitz matrices generated by f. Let $\{E_n\}$ be the sequence of Toeplitz matrices generated by the function*

$$b_\nu(\theta) = [2 - 2\cos(\theta - \theta_0)]^\nu + f_{\min}. \tag{3.23}$$

Then $\kappa(E_n^{-1}T_n)$ is uniformly bounded for all $n > 0$.

Proof. We can assume without loss of generality that $\theta_0 = 0$. Let G_n be generated by $f(\theta + \theta_0)$. The function $f(\theta + \theta_0) - f_{\min}$ has a zero at $\theta = 0$ and

$$G_n = V_n^* T_n V_n,$$

where $V_n = \mathrm{diag}(1, e^{-i\theta_0}, e^{-2i\theta_0}, \cdots, e^{-i(n-1)\theta_0})$, see Chan [14, Lemma 2].

By assumption, there exists a neighborhood N of 0 such that f is continuous in N. Define

$$F(\theta) = \frac{f(\theta)}{(2 - 2\cos\theta)^\nu + f_{\min}}.$$

Clearly F is continuous and positive for $\theta \in N \setminus \{0\}$. Since

$$\lim_{\theta \to 0} F(\theta) = \begin{cases} 1 & f_{\min} > 0, \\ \dfrac{f^{(2\nu)}(0)}{(2\nu)!} & f_{\min} = 0, \end{cases}$$

is positive, F is a continuous positive function in N. Since f is piecewise continuous and positive almost everywhere in $[-\pi, \pi] \setminus N$, we see that F is a piecewise continuous function with a positive essential infimum in $[-\pi, \pi]$. Hence there exist constants $b_1, b_2 > 0$, such that $b_1 \le F(\theta) \le b_2$ almost everywhere in $[-\pi, \pi]$. Without loss of generality, we assume that $b_2 \ge 1 \ge b_1$. Then we have

$$b_1 \le \frac{u^* T_n u}{u^*(E_n + f_{\min} \cdot I_n)u} \le b_2$$

for any n-vector u. Hence $\kappa(E_n^{-1}T_n) \le b_2/b_1$, which is independent of n. □

We note that E_n is a band-Toeplitz matrix with bandwidth $2\nu + 1$ and its diagonals can be obtained by using Pascal's triangle. The band system $E_n y = z$ can be solved by using any band matrix solver, see Golub and Van Loan [50], or Wright [89] for a parallel one. The cost of factorizing E_n is about $\frac{1}{2}\nu^2 n$ operations, and then each subsequent solve requires an extra $(2\nu + 1)n$ operations. Hence, the total number of operations per iteration is of $O(n \log n)$ as ν is independent of n.

When $f_{\min} = 0$, the band preconditioner has improved the condition number from $\kappa(T_n) = O(n^{2\nu})$ to $\kappa(E_n^{-1}T_n) = O(1)$. Since the number of iterations required to attain a given tolerance ϵ is bounded by

$$\frac{1}{2}\sqrt{\kappa(E_n^{-1}T_n)}\log(\frac{2}{\epsilon}) + 1,$$

see for instance [3, p.26], the overall work required to attain the given tolerance is reduced from $O(n^{\nu+1}\log n)$ to $O(n\log n)$ operations. As for the storage, we just need an n-by-$(2\nu+1)$ matrix to hold the factors of the preconditioner E_n. Thus, the overall storage requirement in the conjugate gradient method is about $(8+\nu)n$. Finally, we remark that similar results hold when there are multiple points on $[-\pi, \pi]$ where f takes on its minimum value, see R. Chan [15].

3.2.3. Toeplitz-circulant Preconditioners The main idea behind Theorem 3.2.8 is to approximate the given non-negative generating function f by trigonometric polynomials that match the zeros of f. Clearly, any function g that matches the zeros of f and gives rise to Toeplitz matrices that are easily invertible can be considered too. This idea is exploited in Di Benedetto [4], Di Benedetto, Fiorentino, and Serra [5], R. Chan and Tang [33] and R. Chan and Ching [18]. In [18], they considered using products of circulant matrices and band-Toeplitz matrices as preconditioners for Toeplitz systems generated by non-negative functions. The band-Toeplitz part of these *Toeplitz-circulant preconditioners* is to match the zeros of the given function, and the circulant part is to speed up the convergence rate of the algorithm. Instead of using powers of $2 - 2\cos\theta$ as in (3.45) to generate the band-Toeplitz part of the preconditioner, they considered using powers of $1 - e^{i\theta}$ instead. This results in preconditioners that can handle complex-valued generating functions with zeros of arbitrary orders.

THEOREM 3.2.9. **(R. Chan and W. Ching [18])** *Suppose that $f(z)$ is of the form*

$$f(z) = \left\{\prod_j (z - z_j)^{\ell_j}\right\} h(z), \quad \text{with} \quad z = e^{i\theta}$$

where z_j are the roots of $f(z)$ on $|z| = 1$ with order ℓ_j and $h(z)$ is a non-vanishing function on $|z| = 1$. Let $\{T_n\}$, $\{E_n\}$ and $\{G_n\}$ be sequences of Toeplitz matrices generated by f, $\prod_j (z - z_j)^{\ell_j}$ and h respectively. Then the sequence of matrices $c(G_n)E_n^{-1}T_n$ has singular values clustered around 1 for all sufficiently large n.

Proof. By expanding the product $\prod_j (z - z_j)^{\ell_j}$ we see that the Toeplitz matrix E_n is a lower triangular matrix with band-width equal to $(\ell + 1)$ where $\ell = \sum_j \ell_j$. Moreover, its main diagonal entry is 1 and therefore it is invertible for all n. We see that the matrix $T_n - E_nG_n$ only has non-zero entries in the first $l + 1$ rows. Hence it is clear that

$$T_n = E_nG_n + L_1,$$

where rank $L_1 \le \ell + 1$. Therefore

$$c(G_n)^{-1}E_n^{-1}T_n = c(G_n)^{-1}E_n^{-1}(E_nG_n + L_1) = c(G_n)^{-1}G_n + L_2, \tag{3.24}$$

where rank $L_2 \le \ell$.

Since $h(z)$ has no zeros on $|z| = 1$, the matrices $c(G_n)^{-1}G_n$ has clustered singular values. In particular, we can write $c(G_n)^{-1}G_n = I + L_3 + U$ where U is a small norm matrix and rank L_3 is fixed independent of n. Hence (3.24) becomes

$$E_n^{-1}c(G_n)^{-1}T_n = I + L_4 + U$$

where the rank of L_4 is again fixed independent of n. By using Cauchy interlace theorem [88, p.103] on

$$(E_n^{-1}c(G_n)^{-1}T_n)^*(E_n^{-1}c(G_n)^{-1}T_n) = (I + L_4 + U)^*(I + L_4 + U),$$

it is straightforward to show that $E_n^{-1}c(G_n)^{-1}T_n$ has singular values clustered around 1. □

In each iteration of the PCG method, we have to solve a linear system of the form $E_nc(G_n)y = r$. We first claim that $E_nc(G_n)$ is invertible for large n. As mentioned above, the Toeplitz matrix E_n is invertible for all n. Since h is a Wiener class function and has no zeros on $|z| = 1$, the invertibility of $c(G_n)$ for large n is guaranteed by Theorem 3.2.6. Hence $c(G_n)E_n$ is invertible for large n. Let us consider the cost of solving the system

$$c(G_n)E_ny = r.$$

As the matrix E_n is a lower triangular matrix with band-width $(\ell + 1)$, the system involving E_n can be solved by forward substitution and the cost is $O(\ell n)$ operations. Given any vector x, the matrix-vector product $c(G_n)x$ can be done by using FFTs in $O(n \log n)$ operations. Thus the system $c(G_n)E_ny = r$ can be solved in $O(n \log n) + O(\ell n)$ operations.

3.3. Preconditioners for Linear Systems with Matrix Structure

3.3.1. Toeplitz-like Systems We first briefly review relevant definitions and results on displacement structure representation of a matrix. We introduce the $n \times n$ *lower shift* matrix Z_n, whose entries are zero everywhere except for the 1's on the first subdiagonal, i.e.,

$$Z_n = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & & 0 \\ \vdots & 1 & 0 & \ddots & \vdots \\ 0 & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

The *displacement operator* ∇ is defined by

$$\nabla A_n = A_n - Z_nA_nZ_n^*,$$

where ∇A_n is called the displacement of A_n, cf. Chun and Kailath [40]. Let $L_n(w)$ denote the $n \times n$ lower triangular Toeplitz matrix with first column the vector w.

THEOREM 3.3.1. **(J. Chun, T. Kailath, and H. Lev-Ari [41])** *An arbitrary $n \times n$ matrix A_n can be written in the form*

$$A_n = \sum_{i=1}^{\rho} L_n(u_i) L_n(v_i)^*, \tag{3.25}$$

where $\rho = rank(\nabla A_n)$ and u_i and v_i are n-vectors.

The sum given in Theorem 3.3.1 above is called the *displacement representation* of the given matrix A_n and the scalar ρ is called the *displacement rank* of A_n. Square Toeplitz matrices and Toeplitz-like matrices have small displacement rank, see [41].

For example, a Hermitian Toeplitz matrix $T_n = [t_{i-j}]_{i,j=1}^n$ (where $t_{-r} = \bar{t}_r$) has displacement rank at most 2, since

$$T_n = L_n(x_+) L_n(x_+)^* - L_n(x_-) L_n(x_-)^*,$$

where

$$x_{\pm} = [\frac{1}{2}(t_0 \pm 1), t_1, \cdots, t_{n-1}]^*.$$

To see this, we observe that $x_+ = x_- + e_1$, where $e_1 = [1, 0, \cdots, 0]^*$. Hence

$$x_+ x_+^* - x_- x_-^* = e_1 x_-^* + x_- e_1^* + e_1 e_1^* = \begin{bmatrix} t_0 & t_1 & t_2 & \cdots & t_{n-1} \\ t_1 & & & & \\ t_2 & & 0 & & \\ \vdots & & & & \\ t_{n-1} & & & & \end{bmatrix} = \nabla T_n.$$

If $T_{m,n}$ is an m-by-n Toeplitz matrix with $m \geq n$, then $T_{m,n}^* T_{m,n}$ is in general not a Toeplitz matrix. However $T_{m,n}^* T_{m,n}$ does have a small displacement rank, $\rho \leq 4$, and the displacement representation of $T_{m,n}^* T_{m,n}$ is

$$T_{m,n}^* T_{m,n} = L_n(x_1) L_n(x_1)^* - L_n(x_2) L_n(x_2)^* + L_n(y_1) L_n(y_1)^* - L_n(y_2) L_n(y_2)^*,$$

where

$$x_1 = T_{m,n}^* T_{m,n} e_1 / ||T e_1||, \quad x_2 = Z_n Z_n^* x_1,$$

$$y_1 = [0, t_{-1}, t_{-2}, \cdots, t_{1-n}]^* \quad \text{and} \quad y_2 = [0, t_{m-1}, t_{m-2}, \cdots, t_{m-n+1}]^*.$$

R. Chan, Nagy, and Plemmons [26] and Huckle [58] defined the *displacement preconditioner* to be the circulant approximations of the factors in the displacement representation of A_n in (3.25), i.e., the circulant approximation C_n of A_n is

$$C_n = \sum_{i=1}^{\rho} c(L_n(u_i)) c(L_n(v_i))^*.$$

Recall that $c(X_n)$ is the optimal circulant approximation to X_n in the Frobenius norm, see (3.19). In the following, we assume that the generating function f of $T_{m,n}$ is in the Wiener class, i.e. the diagonals of $T_{m,n}$ are absolutely summable:

$$\sum_{j=-\infty}^{\infty} |t_j| \leq \gamma < \infty. \tag{3.26}$$

R. Chan, Nagy and Plemmons [26] showed that

$$T_{m,n}^* T_{m,n} = T + L(y_1)L(y_1)^* - L(y_2)L(y_2)^* \tag{3.27}$$

where T is a Hermitian Toeplitz matrix with

$$Te_1 \equiv \begin{bmatrix} t_0 \\ t_1 \\ \vdots \\ t_{n-1} \end{bmatrix} = T_{m,n}^* T_{m,n} e_1. \tag{3.28}$$

They also defined the displacement preconditioner for $T_{m,n}^* T_{m,n}$ to be P_n:

$$P_n = c(T) + c(L(y_1))c(L(y_1))^*.$$

In the following, we will show that P_n is a good preconditioner.

For simplicity, we will denote by U_i Hermitian matrices with small rank and V_i Hermitian matrices with small norm. More precisely, given any $\epsilon > 0$, there exist integers N and $M > 0$, such that when n, the size of the matrices U_i and V_i, is larger than N, the rank of U_i is bounded by M and $||V_i||_2 < \epsilon$.

LEMMA 3.3.1.

$$L(y_2)L(y_2)^* = U_1 + V_1. \tag{3.29}$$

Proof. Since the sequence $\{t_j\}_{j=-\infty}^{\infty}$ is absolutely summable, for any given ϵ, we can choose $N > 0$ such that

$$\sum_{j>N} |t_j| < \epsilon.$$

Partition $L(y_2)$ as $R_N + W_N$, where the first N columns of R_N are the first N columns of $L(y_2)$ with the remaining columns zero vectors. Then R_N is a matrix of rank N and

$$||W_N||_1 = \sum_{j=m-n+N+1}^{m-1} |t_j| \leq \sum_{j=N+1}^{m-1} |t_j| < \epsilon.$$

Thus

$$L(y_2)L(y_2)^* = (R_N + W_N)(R_N + W_N)^* = U_1 + V_1,$$

where

$$\text{rank } U_3 = \text{rank}(R_N W_N^* + W_N R_N^* + R_N R_N^*) \leq 2N$$

and

$$||V_3||_2 \leq ||W_N W_N^*||_2 \leq \epsilon^2. \quad \square$$

We note from Lemma 3.3.1 that it suffices to show that the matrix

$$\begin{aligned} & P_n - T_{m,n}^* T_{m,n} \\ = \quad & \{c(T) - T\} + \{c(L(y_1))c(L(y_1))^* - L(y_1)L(y_1)^*\} + L(y_2)L(y_2)^* \end{aligned}$$

is the sum of a matrix of low rank and a matrix of small norm.

THEOREM 3.3.2. **(R. Chan, Nagy and Plemmons [26])** *Let f be a function in the Wiener class. Then the spectra of $P_n - T_{m,n}^* T_{m,n}$ are clustered around zero for large n.*

Proof. The generating function of $T_{m,n}$ is in the Wiener class, therefore the generating function of T is also in the Wiener class. In fact,

$$||Te_1||_1 = ||T_{m,n}^* T_{m,n} e_1||_1 \leq ||T_{m,n}^*||_1 ||T_{m,n} e_1||_1 \leq \gamma^2 < \infty. \tag{3.30}$$

According to Theorem 3.2.3, we have

$$c(T) - T = U_2 + V_2. \tag{3.31}$$

Next we show that

$$c(L(y_1))c(L(y_1))^* - L(y_1)L(y_1)^* = U_3 + V_3 \tag{3.32}$$

The generating function of $L(y_1)$ is given by

$$g(\theta) = \sum_{j=-\infty}^{-1} t_j e^{ij\theta} \tag{3.33}$$

which is a function in the Wiener class. Equation (3.32) now follows by Lemma 5 of [24] or using the arguments in Theorem 3.2.3.

Combining (3.31), (3.32) and (3.29), we see that

$$P_n - T_{m,n}^* T_{m,n} = c(T) - T + c(L(y_1))c(L(y_1))^* - L(y_1)L(y_1)^* + L(y_2)L(y_2)^*$$

is the sum of a matrix of low rank and a matrix of small norm. $\square$

In order to show that $||P_n^{-1}||_2$ is uniformly bounded, we need the following two lemmas. These two lemmas state some properties of the optimal circulant preconditioner for non-Hermitian Toeplitz matrices. Their proofs can be found in [35] and [23] respectively.

LEMMA 3.3.2. *Let $f \in \mathbf{C}_{2\pi}$. Let $\{T_n\}$ be a sequence of Toeplitz matrices generated by f. Then we have*

$$||c(T_n)||_2 \leq 2||f||_\infty, \quad n = 1, 2, \cdots.$$

If moreover f has no zeros, i.e.

$$|f|_{\min} \equiv \min_{\theta \in [-\pi, \pi]} |f(\theta)| > 0,$$

then for all sufficiently large n, we also have

$$||c(T_n)^{-1}||_2 \leq 2||\frac{1}{f}||_\infty.$$

LEMMA 3.3.3. *Let $\{T_n\}$ be a sequence of Toeplitz matrices with generating function in the Wiener class. Then*

$$\lim_{n\to\infty} \|c(T_n)c(T_n)^* - c(T_nT_n^*)\|_2 = 0.$$

We now are ready to show that $\|P_n^{-1}\|_2$ is uniformly bounded.

THEOREM 3.3.3. **(R. Chan, Nagy and Plemmons [26])** *Let the generating function f of $T_{m,n}$ be a Wiener class function that satisfies*

$$\min_{\theta\in[-\pi,\pi]} |f(\theta)| \geq \delta > 0. \tag{3.34}$$

Then $||P_n||_2 \leq 6\gamma^2$ for all n and $||P_n^{-1}||_2$ is uniformly bounded for n sufficiently large.

Proof. We note that

$$||P_n||_2 \leq ||c(T)||_2 + ||c(L(y_1))c(L(y_1))^*||_2 \leq ||T||_2 + ||c(L(y_1))||_2^2.$$

It follows from (3.30) that

$$||T||_2 \leq ||T||_1 \leq 2||Te_1||_1 \leq 2\gamma^2.$$

On the other hand, using Lemma 3.3.2, we have

$$||c(L(y_1))||_2 \leq 2||g||_\infty$$

where g is the generating function of $L(y_1)$ given in (3.33). Thus

$$||c(L(y_1))||_2 \leq 2||\sum_{j=-\infty}^{-1} t_j e^{ij\theta}||_\infty \leq 2\gamma.$$

Since the generating function g of $L(y_1)$ is in the Wiener class, it follows from Lemma 3.3.3 that given any $\epsilon > 0$,

$$c(L(y_1))c(L(y_1))^* - c(L(y_1)L(y_1)^*) = V_4,$$

where $||V_4||_2 < \epsilon$, provided that the size n of the matrix is sufficiently large [23]. Hence

$$\begin{aligned} P_n &= c(T) + c(L(y_1))c(L(y_1))^* = c(T) + c(L(y_1)L(y_1)^*) + V_4 \\ &= c(T + L(y_1)L(y_1)^*) + V_4 = c(T_{m,n}^*T_{m,n} + L(y_2)L(y_2)^*) + V_4, \end{aligned}$$

where the last equality follows from (3.27). Write

$$T_{m,n} = \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

where T_1 is the n-by-n submatrix of $T_{m,n}$. The matrices $T_{m,n}$ and T_1 have the same generating function f and $T_{m,n}^*T_{m,n} = T_1^*T_1 + T_2^*T_2$.

Since f by assumption is in the Wiener class,

$$c(T_1^* T_1) = c(T_1)^* c(T_1) + V_5,$$

where $||V_5||_2 \le \epsilon$ if n is sufficiently large. Thus

$$\begin{aligned} P_n &= c(T_{m,n}^* T_{m,n} + L(y_2)L(y_2)^*) + V_4 \\ &= c(T_1^* T_1 + T_2^* T_2 + L(y_2)L(y_2)^*) + V_4 \\ &= c(T_1)^* c(T_1) + c(T_2^* T_2 + L(y_2)L(y_2)^*) + V_4 + V_5, \end{aligned} \tag{3.35}$$

Observe that

$$\{\lambda_{\min}[c(T_1)^* c(T_1)]\}^{-1} = ||[c(T_1)^* c(T_1)]^{-1}||_2 = ||c(T_1)^{-1}||_2^2 \le 4||\frac{1}{f}||_\infty^2$$

where the last inequality follows from Lemma 3.3.2. Thus by (3.34),

$$\lambda_{\min}[c(T_1)^* c(T_1)] \ge \frac{\delta^2}{4}.$$

Since $T_2^* T_2 + L(y_2)L(y_2)^*$ is a positive semi-definite matrix, $c(T_2^* T_2 + L(y_2)L(y_2)^*)$ is also a positive semi-definite matrix. Thus we conclude from (3.35) that

$$\lambda_{\min}\{P\} \ge \lambda_{\min}[c(T_1)^* c(T_1)] - ||V_4||_2 - ||V_5||_2 \ge \frac{\delta^2}{4} - 2\epsilon.$$

The lemma follows by observing that ϵ is chosen arbitrarily and δ depends only on f and not on n. $\Box$

By combining the above results (Theorems 3.3.2 and 3.3.3), we can show that the spectra of the preconditioned matrices $P_n^{-1} T_{m,n}^* T_{m,n}$ are clustered around one. Thus the conjugate gradient method, when applied to solving the preconditioned system, converges superlinearly. Numerical experiments in [26] show the effectiveness of the preconditioners proposed for Toeplitz least squares problems.

3.3.2. Toeplitz-plus-Hankel Systems The systems of linear equations with Toeplitz-plus-Hankel coefficient matrices arise in many signal processing applications. For example, the inverse scattering problem can be formulated as Toeplitz-plus-Hankel systems of equations, see Gelfand and Levitan [48]. In [64], Ku and Kuo considered an n-by-n Toeplitz-plus-Hankel system $A_n x = b$ where A_n is the sum of a Toeplitz matrix T_n and a Hankel matrix H_n with elements $[T_n]_{i,j} = t_{i-j}$ and $[H_n]_{i,j} = h_{n+1-i-j}$. They proposed using circulant preconditioner to precondition Toeplitz-plus-Hankel matrix $T_n + H_n$.

Let J_n be an n-by-n matrix which has ones along the secondary diagonal and zeros elsewhere, i.e.,

$$J_n = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \iddots & 1 & 0 \\ \vdots & \iddots & \iddots & \iddots & \vdots \\ 0 & 1 & \iddots & \iddots & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix}.$$

It is easy to see that the product of J_n and H_n gives a Toeplitz matrix

$$J_nH_n = \begin{bmatrix} h_0 & h_{-1} & \cdots & h_{2-n} & h_{1-n} \\ h_1 & h_0 & h_{-1} & & h_{2-n} \\ \vdots & h_1 & h_0 & \ddots & \vdots \\ h_{n-2} & & \ddots & \ddots & h_{-1} \\ h_{n-1} & h_{n-2} & \cdots & h_1 & h_0 \end{bmatrix}.$$

We remark that premultiplying J_n to a vector v corresponds to reversing the order of the elements in v. Thus the Hankel matrix-vector products $H_n v$ can be done in $O(n \log n)$ using FFTs. The Toeplitz-plus-Hankel matrix can be expressed as $A_n = T_n + H_n = T_n + J_nJ_nH_n$. Given circulant preconditioners $C_n^{(1)}$ and $C_n^{(2)}$ for Toeplitz matrices T_n and J_nH_n respectively, Ku and Kuo proposed to use

$$P_n = C_n^{(1)} + J_nC_n^{(2)} \tag{3.36}$$

as a preconditioner for the Toeplitz-plus-Hankel matrix $T_n + H_n$.

With the equality $J_n^2 = I_n$ and (3.36), we have

$$P_nz = C_n^{(1)}z + J_nC_n^{(2)}J_nJ_nz = v, \tag{3.37}$$

which is equivalent to

$$J_nP_nz = J_nC_n^{(1)}J_nJ_nz + C_n^{(2)}z = J_nv, \tag{3.38}$$

Since $C_n^{(1)}$ and $C_n^{(2)}$ are circulant,

$$J_nC_n^{(1)}J_n = C_n^{(1)T} \quad \text{and} \quad J_nC_n^{(2)}J_n = C_n^{(2)T}.$$

By multiplying (3.37) with $C_n^{(1)T}$ and (3.38) with $C_n^{(2)T}$, we can write the difference between the two resulting equations as

$$(C_n^{(1)T}C_n^{(1)} - C_n^{(2)T}C_n^{(2)})z = C_n^{(1)T}v - C_n^{(2)T}J_nv. \tag{3.39}$$

The solution of $z = P_n^{-1}v$ can also determined from (3.39). We note that the matrix $C_n^{(1)T}C_n^{(1)} - C_n^{(2)T}C_n^{(2)}$ is circulant and therefore the $P_n^{-1}v$ can be found efficiently via FFT with $O(n \log n)$ operations.

For Toeplitz matrices T_n and J_nH_n generated by rational functions, Ku and Kuo have proved that the spectra of the preconditioned Toeplitz-plus-Hankel matrices are clustered around 1.

THEOREM 3.3.4. **(T. Ku and C. Kuo [64])** *Let $T_n + H_n$ be a real symmetric n-by-n matrix. Let the generating functions of T_n and J_nH_n be*

$$f_1(\theta) = \frac{f_{1,a}(\theta)}{f_{1,b}(\theta)} + \frac{f_{1,c}(\theta)}{f_{1,d}(\theta)} = \frac{\sum_{k=0}^{\alpha_1} a_{1,k}e^{-ik\theta}}{\sum_{k=0}^{\beta_1} b_{1,k}e^{-ik\theta}} + \frac{\sum_{k=0}^{\gamma_1} c_{1,k}e^{ik\theta}}{\sum_{k=0}^{\delta_1} d_{1,k}e^{ik\theta}}$$

and

$$f_2(\theta) = \frac{f_{2,a}(\theta)}{f_{2,b}(\theta)} + \frac{f_{2,c}(\theta)}{f_{2,d}(\theta)} = \frac{\sum_{k=0}^{\alpha_2} a_{2,k}e^{-ik\theta}}{\sum_{k=0}^{\beta_2} b_{2,k}e^{-ik\theta}} + \frac{\sum_{k=0}^{\gamma_2} c_{2,k}e^{ik\theta}}{\sum_{k=0}^{\delta_2} d_{2,k}e^{ik\theta}}$$

with $a_{i,\alpha_i}b_{i,\beta_i}c_{i,\gamma_i}d_{i,\delta_i} \neq 0$, $b_{i,0} = 1$, $d_{i,0} = 1$, *and polynomials* $f_{i,a}(\theta)$ *and* $f_{i,b}(\theta)$, $f_{i,c}(\theta)$ *and* $f_{i,d}(\theta)$ *have no common zeros. If*

$$||\lambda_k(C_n^{(1)})|^2 - |\lambda_k(C_n^{(2)})|^2| \geq \mu > 0, \quad 1 \leq k \leq n$$

where μ *is a constant independent of* n, *then the spectra of* $P_n^{-1}(T_n + H_n)$ *are clustered around 1 and the number of outliers is bounded by*

$$\begin{aligned}\eta \;\; = \;\; & \max\{\max\{\alpha_1,\beta_1\}+\beta_2, \max\{\alpha_2,\beta_2\}+\beta_1\} + \\ & \max\{\max\{\gamma_1,\delta_1\}+\delta_2, \max\{\gamma_2,\delta_2\}+\delta_1\} - \eta_c\end{aligned}$$

where η_c *is the number of common zeros in* $f_{1,b}f_{1,d}$ *and* $f_{2,b}f_{2,d}$.

Using Theorem 3.2.3, we can also prove the following result.

THEOREM 3.3.5. *Let* $T_n + H_n$ *be a real symmetric* n*-by-*n *matrix. Let the generating functions of* T_n *and* J_nH_n *be* f_1 *and* f_2 *respectively. Let* f_1 *and* f_2 *be functions in the Wiener class. If*

$$||\lambda_k(C_n^{(1)})|^2 - |\lambda_k(C_n^{(2)})|^2| \geq \mu > 0, \quad 1 \leq k \leq n$$

where μ *is a constant independent of* n, *then the spectra of* $P_n^{-1}(T_n + H_n)$ *are clustered around 1.*

Proof. Recall from (3.39) that $P_n z = v$ is equivalent to

$$(C_n^{(1)T}C_n^{(1)} - C_n^{(2)T}C_n^{(2)})z = C_n^{(1)T}v - C_n^{(2)T}J_nv.$$

For any given n, $\|C_n^{(1)}\|_1$ and $\|C_n^{(2)}\|_\infty$ are both bounded. As a consequence, $\|C_n^{(1)T}\|_2$ is also bounded. Similar results hold for $C_n^{(2)T}$. Thus the right-hand sides of (3.39) is bounded. Under the assumption, the magnitude of any eigenvalue of $(C_n^{(1)T}C_n^{(1)} - C_n^{(2)T}C_n^{(2)})$ is also bounded. Therefore, $\|P_n^{-1}\|_2$ is bounded and the preconditioner P is invertible.

According to the definitions, the difference matrix $P_n - T_n - H_n$ can be written as

$$P_n - T_n - H_n = (C_n^{(1)} - T_n) + J_n(C_n^{(2)} - J_nH_n).$$

By Theorem 3.2.3, the spectra of the matrices $C_n^{(1)} - T_n$ and and $C_n^{(2)} - J_nH_n$ are clustered around zero for large n. Hence the result follows. □

With the above spectral properties of the preconditioned Toeplitz-plus-Hankel matrices, various preconditioned iterative methods including GMRES and CGS can be effectively applied. These Toeplitz-plus-Hankel systems can be solved in a finite number of iterations independent of n so that total operations required are $O(n \log n)$.

Linear-Phase Filtering Finite impulse response linear-phase filters are commonly used in signal processing. Such filters are especially important for applications where frequency dispersion due to non-linear phase is harmful, such as in speech processing. In this case, the impulse responses can be found by solving the Toeplitz-plus-Hankel least squares problem

$$\min \|\mathbf{d} - (T + H)\mathbf{b}\|_2,$$

where $T + H$ is a rectangular Toeplitz-plus-Hankel matrix, see [67, 68, 69, 90, 56]. By exploiting the structure of the normal equations matrices, it can be written as

$$(T + H)^*(T + H) = \tilde{T}_n + \tilde{H}_n - V_n^{(1)} - V_n^{(2)} - V_n^{(3)} - V_n^{(4)},$$

where $\tilde{T}_n$ is a Toeplitz matrix, $\tilde{H}$ is a Hankel matrix, and $\{V_n^{(i)}\}_{i=1}^4$ are non-Toeplitz and non-Hankel matrices. In [73], the optimal circulant preconditioner $c(\tilde{T}_n)$ is used as a preconditioner for the problem.

We remark that our preconditioner is different from that proposed by Ku and Kuo [64] for Toeplitz-plus-Hankel systems. They basically take the circulant approximations of Toeplitz matrix and Hankel matrix and then combine them together to form a preconditioner. We note that under the assumptions in [64], the spectrum of the Hankel matrix is not clustered around zero. The motivation behind our preconditioner is that the Toeplitz matrix $\tilde{T}_n$ is the sample autocorrelation matrix which intuitively should be a good estimation to the autocorrelation matrix of the discrete-time stationary process, provided that sufficiently large number of data samples are taken. Moreover, under practical signal processing assumptions, the spectrum of the Hankel matrix $\tilde{H}_n$ is clustered around zero. Hence it suffices to approximate $\tilde{T}_n$ by circulant preconditioner.

To prove convergence, the following practical signal processing assumptions of the random process were made, see [73].

- The process is stationary with constant mean μ.
- The spectral density function of the process is positive and in the Wiener class.
- There exist positive constants β_1 and β_2 such that

$$\mathrm{Var}\left(\frac{1}{m}\sum_{j=1}^{m-k} x(j)\right) \le \frac{\beta_1}{m}, \quad k = 0, 1, 2, \ldots, m-1$$

and

$$\mathrm{Var}\left(\frac{1}{m}\sum_{j=1}^{m-k} [x(j) - \mu][x(j+k) - \mu]\right) \le \frac{\beta_2}{m}, \quad k = 0, 1, 2, \ldots, m-1.$$

We note that the positiveness of the spectral density function can be guaranteed by the causality of the process [10, p.85], whereas the absolute summability of the autocovariances can be assured by the invertibility of the process [10, p.86]. With these assumptions, we have proved that the spectra of the preconditioned matrices $c(\tilde{T}_n)^{-1}((T+H)^*(T+H))$ are clustered around 1 with probability 1, provided that a sufficiently large number of data samples are taken.

THEOREM 3.3.6. **(M. Ng [73])** *Let the discrete-time process satisfy the above assumptions. Then for any given $\epsilon > 0$ and $0 < \eta < 1$, there exist positive integers ρ_1 and ρ_2 such that for $n > \rho_1$, the probability that at most ρ_2 eigenvalues of the matrix $I - c(\tilde{T}_n)^{-1}((T+H)^*(T+H))$ have absolute value greater than ϵ is greater than $1-\eta$, provided that $m = O(n^{3+\nu})$ with $\nu > 0$.*

Hence, when we apply the conjugate gradient method to the preconditioned system, the method converges superlinearly with probability 1. Since the data matrix $T+H$ is an m-by-n rectangular matrix, the normal equations and the circulant preconditioner can be formed in $O(m \log n)$ operations. Once they are formed, the cost per iteration of the preconditioned conjugate gradient method is $O(n \log n)$ operations. Therefore, the total work of obtaining the filter coefficients to a given accuracy is of $O((m+n)\log n)$.

Numerical Solutions of Biharmonic Equations Boundary value problems for the biharmonic equation in two dimensions arise in the computation of the Airy stress function for plane stress problems [71], and in steady Stokes flow of highly viscous fluids [70, Chapter 22]. Integral equations method is a popular choice for the numerical solution of these equations [51]. The application of conformal mapping to this problem, though classical, is less well known [71]. Unlike the Laplace equation, the biharmonic equation is not preserved under conformal transplantation. However, a biharmonic function and its boundary values can be represented in terms of the analytic Goursat functions and this representation can be transplanted with a conformal map to a computational region, such as a disk, an ellipse, or an annulus, where the boundary value problem can be solved more easily.

We wish to find a function $u = u(\eta, \mu)$ which satisfies the biharmonic equation,

$$\Delta^2 u = 0,$$

for $\zeta = \eta + i\mu \in \Omega$ where Ω is a region with a smooth boundary Γ and u satisfies the boundary conditions

$$u_\eta = G_1 \quad \text{and} \quad u_\mu = G_2$$

on Γ. The solution u can be represented as

$$u(\zeta) = Re(\overline{\zeta}\phi(\zeta) + \chi(\zeta)),$$

where $\phi(\zeta)$ and $\chi(\zeta)$ are analytic functions in Ω, known as the *Goursat* *functions.* Letting $G = G_1 + iG_2$, the boundary conditions become

$$\phi(\zeta) + \zeta\overline{\phi'(\zeta)} + \overline{\psi(\zeta)} = G(\zeta), \quad \zeta \in \Gamma \tag{3.40}$$

where $\psi(\zeta) = \chi'(\zeta)$. The problem is to find ϕ and ψ satisfying (3.40).

Let $\zeta = f(z)$ be the conformal map from the unit disk to Ω, fixing $f(0) = 0 \in \Omega$. Then with $d(z) \equiv f(z)/\overline{f'(z)}$, $\phi(z) \equiv \phi(f(z)), \psi(z) \equiv \psi(f(z))$, and $G(z) \equiv G(f(z))$, equation (3.40) transplants to the unit disk as

$$\phi(z) + d(z)\overline{\phi'(z)} + \overline{\psi(z)} = G(z), \quad |z| = 1. \tag{3.41}$$

Let

$$\phi(z) = \sum_{k=1}^{\infty} a_k z^k \quad \text{and} \quad \psi(z) = \sum_{k=0}^{\infty} b_k z^k.$$

The problem now is to find the a_k's and the b_k's. For $|z| = 1$, define the Fourier series

$$d(z) := f(z)/\overline{f'(z)} = \sum_{k=-\infty}^{\infty} h_k z^k, \quad G(z) = \sum_{k=-\infty}^{\infty} A_k z^k. \tag{3.42}$$

Substituting (3.42) into (3.41) gives a linear system of equations for the a_k's and b_k's,

$$a_j + \sum_{k=1}^{\infty} k\overline{a}_k h_{k+j-1} = A_j, \quad j = 1, 2, 3, \ldots \tag{3.43}$$

$$\overline{b}_j + \sum_{k=1}^{\infty} k\overline{a}_k h_{k-j-1} = A_{-j}, \quad j = 0, 1, 2, \ldots \tag{3.44}$$

If (3.43) is solved for the a_k's, then the b_k's can be easily computed from (3.44). These systems are derived in [71]. We note that the coefficient matrix of the (infinite) linear system in (3.43) is of the form $I + HD$ where I is the identity matrix, D a diagonal matrix, and H is a Hankel matrix. We remark that HD actually can be represented as a compact operator with a one dimensional null space, see [20].

In [20], the linear system in (3.43) was truncated after n terms and solved efficiently using the conjugate gradient method (up to the null vector). To solve the discrete system, one major computations required at each iteration are the matrix-vector products $H_n v$ with an arbitrary vector v. We note that the Hankel matrix-vector products $H_n v$ can be done in $O(n \log n)$ using FFTs.

For the convergence rate of the conjugate gradient method, estimates are given in [21] for the decay rates of the eigenvalues of the compact operators when the boundary curve is analytic or in a Hölder class. These estimates are used to give detailed bounds for the r-superlinear convergence which do not depend on the right hand side. It follows that the conjugate gradient method, when applied to solve this kind of Hankel systems, converges sufficiently fast.

THEOREM 3.3.7. **(R. Chan, T. DeLillo, and M. Horn [21])** *Assume that the coefficient matrix A_∞ in the infinite linear system (3.43) is positive* *semidefinite with exactly one null vector v. Then, for large n, the error vector e_q at the qth step of the conjugate gradient method applied to $v^{(n)\perp}$ satisfies the following estimates.*

(i) If Γ is analytic, there is an r, $0 < r < 1$, such that

$$|||e_{4q}||| \leq C^q r^{q^2} |||e_0|||.$$

(ii) If Γ is of class $C^{l+1,\alpha}$, $l \geq 2$, $0 < \alpha < 1$, then

$$|||e_{4q}||| \leq \frac{C^q}{((q-1)!)^{2(l-2+\alpha)}} |||e_0|||.$$

Here C is a constant that depends on the conformal map.

The proof follows closely the proof of Theorem 3.2.4. In case A_∞ is not semidefinite we can solve the normal equations by the conjugate gradient method. It is clear that $(I_n + A_n)^2$ will then be positive definite on $\underline{v}^{(n)\perp}$. A similar result for the normal equations can be established. For a discussion of the numerical conformal mapping methods used, see [20].

3.3.3. Toeplitz-plus-band Systems In this subsection, we consider the solution of systems of the form $(T_n + B_n)x = b$, where T_n is an n-by-n Hermitian Toeplitz matrix and B_n is an n-by-n Hermitian band matrix with band-width $2b+1$ independent of n. These systems appear in solving Fredholm integro-differential equations of the form

$$L\{x(\theta)\} + \int_\alpha^\beta K(\phi - \theta)x(\phi)d\phi = b(\theta).$$

Here $x(\theta)$ is the unknown function to be found, $K(\theta)$ is a convolution kernel, L is a differential operator and $b(\theta)$ is a given function. After discretization, K will lead to a Toeplitz matrix, L a band matrix and $b(\theta)$ the right hand side vector, see Delves and Mohamed [47, p.343]. Toeplitz-plus-band matrices also appear in signal processing literature and have been referred to as periheral innovation matrices, see Carayannis et. al. [12].

Unlike Toeplitz systems, there exist no fast direct solvers for solving Toeplitz-plus-band systems. It is mainly because the displacement rank of the matrix $T_n + B_n$ can take any value between 0 and n. Hence, fast Toeplitz solvers that are based on small displacement rank of the matrices cannot be applied. Conjugate gradient methods with circulant preconditioners do not work for Toeplitz-plus-band systems either. In fact, Strang's circulant preconditioner is not even defined for non-Toeplitz matrices. T. Chan's circulant preconditioner, while defined for $T_n + B_n$, does not work well when the eigenvalues of B_n are not clustered, see [27]. Also, the matrix $c(T_n) + B_n$ cannot be used as a preconditioner for it cannot be inverted easily.

In [27], Chan and Ng proposed using the matrix $E_n + B_n$ to precondition $T_n + B_n$ where E_n is the band-Toeplitz preconditioner. Recall that a function f

is said to have a νth order zero at θ_0 if $f(\theta_0)=0$ and ν is the smallest positive integer such that $f^{(\nu)}(\theta_0)\neq 0$ and $f^{(\nu+1)}(\theta)$ is continuous in a neighborhood of θ_0. With the knowledge of the order of f at its minimum, we can give a better estimate of the spectrum of T_n than that in (3.3).

THEOREM 3.3.8. **(R. Chan and M. Ng [27])** *Let f be a non-negative piecewise continuous real-valued function defined on $[-\pi,\pi]$. Let T_n be generated by f. Suppose that $f(\theta)-f_{\min}$ has a unique zero of order 2ν at $\theta=\theta_0$. Let $\{E_n\}$ be the sequence of Toeplitz matrices generated by the function*

$$b_\nu(\theta)=[2-2\cos(\theta-\theta_0)]^\nu+f_{\min}. \tag{3.45}$$

Then $\kappa((E_n+B_n)^{-1}(T_n+B_n))$ is uniformly bounded for all $n>0$.

We note that E_n is a band matrix with bandwidth $2\nu+1$ and its diagonals can be obtained by using Pascal's triangle. The band system $(E_n+B_n)y=z$ can be solved by using any band matrix solver, see Golub and Van Loan [50], or Wright [89] for a parallel one. Let

$$\gamma=\max\{\nu,b\}.$$

The cost of factorizing E_n+B_n is about $\frac{1}{2}\gamma^2 n$ operations, and then each subsequent solve requires an extra $(2\gamma+1)n$ operations. Hence, the total number of operations per iteration is of $O(n\log n)$ as ν is independent of n. Since the number of iterations required to attain a given tolerance ϵ is bounded by

$$\frac{1}{2}\sqrt{\kappa((E_n+B_n)^{-1}(T_n+B_n))}\log(\frac{2}{\epsilon})+1,$$

see for instance [3, p.26], the overall work required to attain the given tolerance is reduced from $O(n^{\nu+1}\log n)$ to $O(n\log n)$ operations. As for the storage, we just need an n-by-$(2\gamma+1)$ matrix to hold the factors of the preconditioner E_n+B_n. Thus, the overall storage requirement in the conjugate gradient method is about $(8+\gamma)n$.

3.3.4. Queueing Networks with Batch Arrivals In this subsection, we consider using the PCG method with the Toeplitz-circulant preconditioners (see §3.2.3) for solving the stationary probability distribution vectors for Markovian queueing models with batch arrivals. This kind of queueing system occurs in many applications, such as telecommunication networks [76] and loading dock models [78]. We will see that the generator matrices of these systems have a near-Toeplitz structure and our preconditioners are constructed by exploiting this fact.

Let us first introduce the following queueing parameters. Definitions of queueing theory terminologies used below can be found in Cooper [44]. The input of the queueing system will be an exogenous Poisson batch arrival process with mean batch inter-arrival time λ^{-1}. For $k\geq 1$, denote λ_k to be the batch arrival rate for batches with size k. We note that

$$\lambda_k=\lambda p_k \tag{3.46}$$

here p_k is the probability that the arrival batch size is k. Clearly we have

$$\sum_{k=1}^{\infty} \lambda_k = \lambda. \tag{3.47}$$

The number of servers in the queueing system will be denoted by s. The service time of each server is independent of the others and is exponentially distributed with mean μ^{-1}. The waiting room is of size $(n-s-1)$ and the queueing discipline is blocked customers cleared. If the arrival batch size is larger than the number of waiting places left, then only part of the arrival batch will be accepted; the other customers will be treated as overflows and will be cleared from the system.

By ordering the state-space lexicographically, i.e. the i-th variable corresponds to the state where there are $(i-1)$ customers in the system, the queueing model can be characterized by the infinitesimal generator matrix

$$A_n = \begin{bmatrix} \lambda & -\mu & 0 & 0 & 0 & \ldots & 0 \\ -\lambda_1 & \lambda+\mu & -2\mu & 0 & 0 & \ldots & 0 \\ -\lambda_2 & -\lambda_1 & \lambda+2\mu & \ddots & \ddots & & \vdots \\ \vdots & -\lambda_2 & \ddots & \ddots & -s\mu & \ddots & \\ & \vdots & \ddots & \ddots & \lambda+s\mu & \ddots & 0 \\ -\lambda_{n-2} & -\lambda_{n-3} & & & \vdots & \lambda+s\mu & -s\mu \\ -r_1 & -r_2 & -r_3 & \cdots & -r_{s+1} & \cdots & s\mu \end{bmatrix}, \tag{3.48}$$

where r_i are such that each column sum of A_n is zero, see Seila [78].

Clearly A_n has zero column sum, positive diagonal entries and non-positive off diagonal entries. Moreover the matrix A_n is irreducible. In fact, if $\lambda_i = 0$ for all $i = 1, \ldots, n-2$, then $r_1 = \lambda$ and the matrix is irreducible. If the λ_i's are not all zero, say λ_j is the first nonzero λ_i, then $r_{n-j} = \lambda$, and hence A_n is also irreducible. From Perron and Frobenius theory [86, p.30], A_n has a 1-dimensional null-space with a positive null vector.

The stationary probability distribution vector p of the queueing system is the normalized null-vector of the generator matrix A_n given in (3.48). Many useful information about the queueing system, such as the blocking probability and the expected waiting time of customers can be obtained from p. Since A_n has a 1-dimensional null-space, p can be found by deleting the last column and the last row of A_n and solving the $(n-1)$-by-$(n-1)$ reduced linear system $Q_{n-1}y = (0, \ldots, 0, s\mu)^T$. After getting y, the distribution vector p can then be obtained by normalizing the vector $(y^T, 1)^T$.

Thus let us concentrate ourselves in solving nonhomogeneous systems of the form

$$Q_n x = b \tag{3.49}$$

where

$$
(3.50)\quad Q_n = \begin{bmatrix}
\lambda & -\mu & 0 & 0 & 0 & \dots & 0 \\
-\lambda_1 & \lambda+\mu & -2\mu & 0 & 0 & \dots & 0 \\
-\lambda_2 & -\lambda_1 & \lambda+2\mu & \ddots & \ddots & & \vdots \\
\vdots & -\lambda_2 & \ddots & \ddots & -s\mu & \ddots & \\
 & \vdots & \ddots & \ddots & \lambda+s\mu & \ddots & 0 \\
-\lambda_{n-2} & -\lambda_{n-3} & & \ddots & \ddots & \ddots & -s\mu \\
-\lambda_{n-1} & -\lambda_{n-2} & & \dots & -\lambda_2 & -\lambda_1 & \lambda+s\mu
\end{bmatrix}.
$$

Notice that if all of the λ_i, $i = 1, \dots, n-1$ are zeros, then Q_n will be a bidiagonal matrix and can easily be inverted. Therefore in the following, we assume that at least one of the λ_i is non-zero. Then clearly, Q_n^T is an irreducibly diagonally dominant matrix. In particular, if the system (3.49) is solved by classical iterative methods such as the Jacobi or the Gauss-Seidel methods, both methods will converge for arbitrary initial guesses, see for instance Varga [86, Theorem 3.4].

We see that the costs per iteration of the Jacobi and the Gauss-Seidel methods are $O(n \log n)$ and $O(n^2)$ respectively. The memory requirement is $O(n)$ for both methods. We remark that the system (3.49) can also be solved by Gaussian elimination in $O(n^2)$ operations with $O(n^2)$ memory. In the remaining of this subsection, we are interested in solving (3.49) by the PCG method. We will see that the cost per iteration of the method is $O(n \log n)$ and memory requirement is $O(n)$, the same as those of the Jacobi method.

However, we are able to show that if s is independent of n, then with our Toeplitz-circulant preconditioner, the PCG method converges superlinearly for all sufficiently large n. In particular, the method converges in finite number of steps independent of the queue size n. Therefore the total cost of finding the steady-state probability distribution is $O(n \log n)$ operations.

We observe that in the single server case, i.e. when $s = 1$, the matrix Q_n given in (3.50) differs from a lower Hessenberg Toeplitz matrix by only its $(1,1)$ entry. In general, Q_n can be written as

$$
(3.51)\qquad Q_n = T_n + R_n,
$$

where T_n is a Toeplitz matrix:

$$
(3.52)\quad T_n = \begin{bmatrix}
\lambda+s\mu & -s\mu & 0 & 0 & 0 & \dots & 0 \\
-\lambda_1 & \lambda+s\mu & -s\mu & 0 & 0 & \dots & 0 \\
-\lambda_2 & -\lambda_1 & \lambda+s\mu & \ddots & \ddots & & \vdots \\
\vdots & -\lambda_2 & \ddots & \ddots & -s\mu & \ddots & \\
 & \vdots & \ddots & \ddots & \lambda+s\mu & \ddots & 0 \\
-\lambda_{n-2} & & & \ddots & \ddots & \ddots & -s\mu \\
-\lambda_{n-1} & -\lambda_{n-2} & & \dots & -\lambda_2 & -\lambda_1 & \lambda+s\mu
\end{bmatrix},
$$

and R_n is a matrix of rank s.

From (3.52), we see that T_n is generated by $g(z)$ given by

$$g(z) = -s\mu\frac{1}{z} + \lambda + s\mu - \sum_{k=1}^{\infty} \lambda_k z^k \tag{3.53}$$

with $z = e^{i\theta}$. We note that by (3.47), $g(z)$ belongs to the Wiener class of functions defined on the unit circle $|z| = 1$. Unfortunately, it is also clear from (3.53) and (3.47) that $g(z)$ has a zero at $z = 1$. If we look at the real part of $g(z)$ on the unit circle $|z| = 1$, we see that

$$\mathrm{Re}\{g(z)\} = -s\mu\cos\theta + \lambda + s\mu - \sum_{k=1}^{\infty} \lambda_k \cos(k\theta) \geq s\mu - s\mu\cos\theta.$$

Hence the zeros of $g(z)$ can only occur at $z = 1$. In particular, we can write

$$g(z) = (z-1)^{\ell} b(z), \tag{3.54}$$

where ℓ is the order of the zero of $g(z)$ at $z = 1$ and $b(z)$ will have no zeros on the unit circle.

Using the idea developed in §3.2.3, we define our preconditioner for Q_n as

$$P_n = E_n c(G_n) \tag{3.55}$$

where E_n and G_n are the Toeplitz matrices generated by $(z-1)^{\ell}$ and $b(z)$ respectively and $c(G_n)$ is the optimal circulant approximation of G_n.

Let us consider cases where the quotient function $b(z)$ will be a Wiener class function and $b(z)$ has no zeros on $|z| = 1$. We first note that if the radius of convergence ρ of the power series $\sum_{k=1}^{\infty} \lambda_k z^k$ in (3.53) is greater than 1, then $g(z)$ and hence $b(z)$ are analytic functions in a neighborhood of $|z| = 1$, see Conway [42, p.31]. In particular, $b(z)$ will be a Wiener class function and $b(z)$ has no zeros on $|z| = 1$. A formula for computing ρ is given by

$$\frac{1}{\rho} = \limsup |\lambda_j|^{1/j}, \tag{3.56}$$

see Conway [42, p.31].

Next we consider the case $\ell = 1$ in more depth. By straightforward division of $g(z)$ in (3.53) by $(z-1)$, we have

$$b(z) = s\mu\frac{1}{z} - \lambda - \sum_{k=1}^{\infty} (\lambda - \sum_{j=1}^{k} \lambda_j) z^k. \tag{3.57}$$

Therefore, by (3.46) and (3.47),

$$b(1) = s\mu - \sum_{k=0}^{\infty} \sum_{j=k+1}^{\infty} \lambda_j = s\mu - \lambda \sum_{k=0}^{\infty} k p_k = s\mu - \lambda \mathcal{E}(B) \tag{3.58}$$

where $\mathcal{E}(B)$ is the expected value of the arrival batch size. Thus if $s\mu \neq \lambda\mathcal{E}(B)$ then $b(1) \neq 0$ and hence $\ell = 1$. Moreover, if $\mathcal{E}(B) < \infty$, then $b(z)$ is again a Wiener class function and $b(z)$ has no zeros on $|z| = 1$. Clearly from (3.57), the first n Laurent coefficients of $b(z)$, i.e. $\sum_{j=1}^{k} \lambda_j - \lambda$, $k = 1, 2, \ldots, n$, can be computed recursively in $O(n)$ operations. Hence by using (3.19), $c(G_n)$ and also P_n can be constructed in $O(n)$ operations.

THEOREM 3.3.9. **(R. Chan and W. Ching [18])** *Let $b(z)$ be defined as in (3.54) and the number of servers s in the queue be independent of the queue size n. Then the sequence of preconditioned matrices $P_n^{-1}Q_n$ has singular values clustered around* 1 *for large n.*

Proof. By (3.51) and (3.55),

$$P_n^{-1}Q_n = c(G_n)^{-1}E_n^{-1}(T_n + R_n) = c(G_n)^{-1}E_n^{-1}T_n + L_n$$

where rank $L_n \leq s$. Using Theorem 3.2.9, we can show that the sequence of matrices $c(G_n)^{-1}E_n^{-1}T_n$ has singular values clustered around 1 for all sufficiently large n. Therefore, the matrix $P_n^{-1}Q_n$ has singular values clustered around 1 for sufficiently large n. □

It follows from standard convergence theory of the PCG method that the method will converge superlinearly and in particular in finite number of steps independent of n. In each iteration of the PCG method, the main computational cost consists of solving a linear system $P_n y = r$ and multiplying Q_n to some vector r. We first recall from §3.2.3 that the cost of solving $P_n y = r$ is of $O(n \log n) + O(\ell n)$ operations. To compute $Q_n r$, we make use of the partitioning (3.51). Note that R_n in (3.51) is a matrix containing only $2s - 1$ nonzero entries, we therefore need $O(s)$ operations for computing $R_n r$. Since T_n is a Toeplitz matrix, $T_n r$ can be computed in $O(n \log n)$ operations by embedding T_n into a $2n$-by-$2n$ circulant matrix, see Strang [79]. Hence $Q_n r$ can be obtained in $O(n \log n)$ operations. Thus the number of operations required for each iteration of the PCG method is of order $O(n \log n)$.

Finally, we consider the memory requirement. We note that besides some n-vectors, we only have to store the first column (or eigenvalues) of the matrices E_n, and $c(G_n)$ but not the whole matrices. Thus we need $O(n)$ memory for the PCG method.

We remark that circulant-type preconditioners has also been used in solving Markovian network with overflow [19] and Markov-modulated Poisson process queueing systems [38].

3.3.5. Image Restorations Image restoration refers to the removal or reduction of degradations (or blur) in an image using a priori knowledge about the degradation phenomena; see for instance [59]. When the quality of the images is degraded by blurring and noise, important information remains hidden and cannot be directly interpreted without numerical processing. In operator notation, the form of the image restoration problem is given as $z = \mathcal{A}u + \eta$, where the operator $\mathcal{A}$ represents the degradation, z is the observed image and η represents an additive noise. Given z and $\mathcal{A}$, and possibly, the statistics of the noise vector η, the problem is to compute an approximation to the original signal u. In many practical applications, the degradation is *spatially invariant*, i.e., it acts uniformly across the image and object planes. In this case, the discretization of $\mathcal{A}$ is just a block-Toeplitz-Toeplitz-block (BTTB) matrix.

Because of the ill-conditioning of $\mathcal{A}$, naively solving $\mathcal{A}u = z$ will lead to extreme instability with respect to perturbations in b, see [59]. The method of *regularization* can be used to achieve stability for these problems [1]. In the classical *Tikhonov regularization* [53], stability is attained by introducing a regularization functional $\mathcal{R}$, which restricts the set of admissible solutions. Since this causes the regularized solution to be biased, a scalar μ, called a regularization parameter, is introduced to control the degree of bias. Specifically, the regularized solution is computed as

$$\min_u \|\mathcal{A}u - z\|_2^2 + \mu\mathcal{R}(u) \tag{3.59}$$

where $\mathcal{R}(\cdot)$ is a certain functional which measures the irregularity of x in a certain sense. When $\mathcal{R}(f) = \|\mathcal{D}_k f\|_2^2$, where D_k is the kth order differential operator, it forces the solution to have a small kth order derivative. Notice that if the discretization of the differential operator is a Toeplitz matrix, then in digital implementation, (3.59) reduces to a block-Toeplitz least squares problem. For these Toeplitz least squares problems, R. Chan, Nagy, and Plemmons [24, 25] and R. Chan, Ng and Plemmons [30] considered different preconditioners based on the circulant approximations. In [30, 72], restoration of real images by using the circulant preconditioned conjugate gradient algorithm has been carried out.

The algorithms for deblurring and noise removal have been based on least squares. The output of these least squares based algorithms will be a continuous or smooth function, which cannot obviously be a good approximation to original image if the original image contains edges. To overcome this difficulty, a technique based on the minimization of the *"total variation norm"* subject to some noise and blurring constraints is proposed by Rudin, Osher and Fatemi [77]. The idea is to use as regularization function the so-called total variation norm:

$$TV(f) = \int_\Omega |\nabla f| \, dxdy = \int_\Omega \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 + \left(\frac{\partial f}{\partial y}\right)^2} \, dxdy.$$

The solution to (3.59) with $R(f) = TV(f)$ can have discontinuities, thus allowing us to recover the edges of the original image from the blurred and noisy data. At a stationary point of (3.59), the gradient vanishes, giving:

$$\begin{aligned} g(u) \equiv \mathcal{A}^*(\mathcal{A}u - z) - \alpha\nabla \cdot \left(\frac{\nabla u}{|\nabla u|}\right) &= 0, \qquad x \in \Omega, \\ \frac{\partial u}{\partial n} &= 0, \qquad x \in \partial\Omega. \end{aligned} \tag{3.60}$$

The second term in g is obtained by taking the gradient of $\alpha \int_\Omega |\nabla u| dx$ and then applying integration by parts from which Neumann boundary condition results. Since the gradient equation of (3.59) is nonlinear, Vogel and Oman [87] employed the fixed point (FP) iteration to solve this nonlinear gradient equation. The FP iteration will produce a sequence of approximations x_k to the solution x and can be expressed as

$$(T^*T + \mu L(x_k))x_{k+1} = T^*b, \quad k = 0, 1, \ldots \tag{3.61}$$

The coefficient matrices T and L correspond to the discretization of the convolution operator and the elliptic operator respectively in the gradient equation (3.60). In [17], R. Chan, T. Chan and C. Wong have used the optimal cosine transform based preconditioner to precondition the linear system. Numerical results showed that the performance of these preconditioners works very well. However, we remark that this is still an active research area in finding good preconditioner for this linearized equation (3.61).

3.4. Concluding Remarks

The conjugate gradient method coupled with a suitable preconditioner can solve a large class of n-by-n linear systems with matrix structure in $O(n \log n)$ operations. This paper summarizes some of the developments of this iterative method for solving Toeplitz-like, Toeplitz-plus-Hankel and Toeplitz-plus-band systems in the past few years. The results show that the method in some instances works better than traditional methods used specifically for these problems. In practical applications, many linear systems with matrix structure arise. For instance, in image processing, the restoration of images in nonlinear space-invariant systems involves the solutions of Toeplitz-like-plus-band systems, see [82]. Iterative methods provide attractive alternatives to solving these large-scale linear systems with matrix structure.

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