Multigrid Method for Ill-Conditioned Symmetric Toeplitz Systems

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Abstract

In this paper, we consider solutions of Toeplitz systems $A_n u = b$ where the Toeplitz matrices A_n are generated by nonnegative functions with zeros. Since the matrices A_n are ill-conditioned, the convergence factor of classical iterative methods, such as the damped Jacobi method, will approach 1 as the size n of the matrices becomes large. Here we propose to solve the systems by the multigrid method. The cost per iteration for the method is of $O(n \log n)$ operations. For a class of Toeplitz matrices which includes weakly diagonally dominant Toeplitz matrices, we show that the convergence factor of the two-grid method is uniformly bounded below 1 independent of n and the full multigrid method has convergence factor depends only on the number of levels. Numerical results are given to illustrate the rate of convergence.

Key Words: Multigrid Method, Toeplitz Matrices.

1 Introduction

In this paper we discuss the solutions of ill-conditioned symmetric Toeplitz systems $A_n u = b$ by the multigrid method. The n-by-n matrices A_n are Toeplitz matrices with generating functions f that are nonnegative even functions. More precisely, the matrices A_n are constant along their diagonals with their diagonal entries given by the Fourier coefficients of f:

$$[A_n]_{j,k} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-i(j-k)\theta} d\theta, \qquad 0 \le j, k < n.$$

Since f are even functions, we have $[A_n]_{j,k} = [A_n]_{k,j}$ and A_n are symmetric.

In [10, pp.64–65], it is shown that the eigenvalues $\lambda_j(A_n)$ of A_n lie in the range of $f(\theta)$, i.e.

$$\min_{\theta \in [-\pi,\pi]} f(\theta) \le \lambda_j(A_n) \le \max_{\theta \in [-\pi,\pi]} f(\theta), \qquad 1 \le j \le n. \tag{1}$$

Moreover, we also have

$$\lim_{n\to\infty} \lambda_{\max}(A_n) = \max_{\theta \in [-\pi,\pi]} f(\theta) \qquad \text{and} \qquad \lim_{n\to\infty} \lambda_{\min}(A_n) = \min_{\theta \in [-\pi,\pi]} f(\theta).$$

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Consequently, if $f(\theta)$ is nonnegative and vanishes at some points $\theta_0 \in [-\pi, \pi]$, then the condition number $\kappa(A_n)$ of A_n is unbounded as n tends to infinity, i.e. A_n is ill-conditioned. In fact, if the zeros of f are of order μ, then $\kappa(A_n)$ grows like $O(n^\mu)$, see for instance [4].

Superfast direct methods for Toeplitz matrices have been developed around 1980. They can solve n-by-n Toeplitz systems in $O(n \log^2 n)$ operations, see for instance [1]. However, their stability properties for ill-conditioned Toeplitz matrices are still unclear. Iterative methods based on the preconditioned conjugate gradient method were proposed in 1985, see [11, 13]. With circulant matrices as preconditioners, the methods require $O(n \log n)$ operations per iteration. For Toeplitz systems generated by positive functions, these methods have shown to converge superlinearly. However, circulant preconditioners in general cannot handle Toeplitz matrices generated by functions with zeros, see the numerical results in §6. The band-Toeplitz preconditioners proposed in [4, 5] can handle functions with zeros, but are restricted to the cases where the order of the zeros are even numbers. Thus they are not applicable for functions like $f(\theta) = |\theta|$. We remark that the cost per iteration of the preconditioned conjugate gradient method with band-Toeplitz preconditioners is also of the order $O(n \log n)$ operations.

Classical iterative methods such as the Jacobi or Gauss-Seidel methods are also not applicable when the generating functions have zeros. Since $\lim_{n\to\infty} \kappa(A_n) = \infty$, the convergence factor is expected to approach 1 for large n. In [8, 9], Fiorentino and Serra proposed to use multigrid method coupled with Richardson method as smoother for solving Toeplitz systems. Their numerical results show that the multigrid method gives very good convergence rate for Toeplitz systems generated by nonnegative functions. The cost per iteration of the multigrid method is of $O(n \log n)$ operations which is of the same order as the preconditioned conjugate gradient methods with either circulant preconditioners or band-Toeplitz preconditioners.

However, in [8, 9], the convergence of the two-grid method (TGM) on first level is only proved for the so-called band τ matrices. These are band matrices that can be diagonalized by sine transform matrices. A typical example is the 1-dimensional discrete Laplacian matrix $\text{diag}[-1, 2, -1]$. In general, τ matrices are not Toeplitz matrices and vice versa. The proof of convergence of the TGM for Toeplitz matrices was not given there.

From the computational point of view, the matrix on the coarser grid in TGM is still too expensive to invert. One therefore usually does not use TGM alone but instead applies the idea of TGM recursively on the coarser grid to get down to the coarsest grid. The resulting method is the full multigrid method (MGM). We remark that the convergence of MGM for Toeplitz matrices or for τ matrices was not discussed in [8, 9].

In this paper, we consider the use of MGM for solving ill-conditioned Toeplitz systems. Our interpolation operator is constructed according to the position of the first non-zero entry on the first row of the given Toeplitz matrix and is different from the one proposed by Fiorentino and Serra [8, 9]. We show that for a class of ill-conditioned Toeplitz matrices which includes weakly diagonally dominant Toeplitz matrices, the convergence factor of TGM with our interpolation operator is uniformly bounded below 1 independent of n. We also prove that for this class of Toeplitz matrices, the convergence factor of MGM with V-cycles will be level-dependent. One standard way of removing the level-dependence is to use "better" cycles such as the F- or the W-cycles, see [12]. We remark however that our numerical results show that MGM with V-cycles already gives level-independent convergence. Since the cost per iteration is of $O(n \log n)$ operations, the total cost of solving the system is therefore of $O(n \log n)$ operations.

We note that the class of functions that we can handle includes functions with zeros of order 2 or less and also functions such as $f(\theta) = |\theta|$ which cannot be handled by band-Toeplitz preconditioners proposed in [4, 5]. We will also give examples of functions that can be handled by multigrid method with our interpolation operator but not with the interpolation operator proposed in [8].

The paper is organized as follows. In §2, we introduce the two-grid method and the full multigrid method. In §3, we analyze the convergence rate of two-grid method. We first establish in §3.1 the convergence of two-grid method on the first level for the class of weakly diagonally dominant Toeplitz matrices. The interpolation operator for these matrices can easily be identified. Then in §3.2, we consider a larger class of Toeplitz matrices which are not necessarily diagonally dominant. The convergence of full multigrid method is studied in §4 by establishing the convergence of the two-grid method on the coarser levels. In §5, we give the computational cost of our method. Numerical results are given in §6 to illustrate the effectiveness of our method. Finally, concluding remarks are given in §7.

2 Multigrid Methods

Given a Toeplitz system $A_n u = b$ with $u \in \mathbb{R}^n$, we define a sequence of sub-systems on different levels:

$$A^m u^m = b^m, \quad u^m \in \mathbb{R}^{n_m}, \quad 1 \le m \le q.$$

Here q is the total number of levels with $m = 1$ being the finest level. Thus for $m = 1$, $A^1 = A_n$ and $n_1 = n$. For $m > 1$, n_m are just the size of the matrix A^m. We denote the interpolation and restriction operators by $I_{m+1}^m : \mathbb{R}^{n_{m+1}} \longrightarrow \mathbb{R}^{n_m}$ and $I_m^{m+1} : \mathbb{R}^{n_m} \longrightarrow \mathbb{R}^{n_m}$ respectively. We will choose

$$I_m^{m+1} = (I_{m+1}^m)^T.$$

The coarse grid operators are defined by the Galerkin algorithm, i.e.

$$A^{m+1} = I_m^{m+1} A^m I_{m+1}^m, \quad 1 \le m \le q. \tag{2}$$

Thus, if A^m is symmetric and positive definite, so is A^{m+1}. The smoothing operator is denoted by $G^m : \mathbb{R}^{n_m} \longrightarrow \mathbb{R}^{n_m}$. Typical smoothing operators are the Jacobi, Gauss-Seidel and Richardson iterations, see for instance [3]. Once the above components are fixed, a multigrid cycling procedure can be set up. Here we concentrate on the V-cycle scheme which is given as follows, see [3, p.48].

```
procedure MGM(ν1,ν2)(u^m, b^m);
          if m = q,
                then u^q := (A^q)^{-1} b^q;
          endif;
          begin do i := 1 to ν1
                    u^m := G^m u^m + (I^{n_m} - G^m)(A^m)^{-1} b^m;
                endo;
                d^{m+1} := I_m^{m+1}(A^m u^m - b^m);
                e_0^{m+1} := 0;
                e^{m+1} := MGM(ν1,ν2)(e_0^{m+1}, d^{m+1});
                u^m := u^m - I_{m+1}^m e^{m+1};
                do i := 1 to ν2
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$$u^m := G^m u^m + (I^{n_m} - G^m)(A^m)^{-1} b^m;$$

`endo;`

$\mathbf{MGM}(\nu_1, \nu_2) := u^m;$

`end;`

Here I^{n_m} is the n_m-by-n_m identity matrix. If we set $q = 2$, the resulting multigrid method is the two-grid method (TGM).

3 Convergence of TGM for Toeplitz Matrices

In this section, we discuss the convergence of TGM for Toeplitz matrices. We first give an estimate of the convergence factor for Toeplitz matrices that are weakly diagonally dominant. Then we extend the results to a larger class of Toeplitz matrices.

Let us begin by introducing the following notations. We say $A > B$ (respectively $A \geq B$) if $A - B$ is a positive (respectively semi-positive) definite matrix. In particular, $A > 0$ means that A is positive definite. The spectral radius of A is denoted by $\rho(A)$. For $A > 0$, we define the following inner products which are useful in the convergence analysis of multigrid methods, see [12, p.77–78]:

$$\langle u, v\rangle_0 = \langle \mathrm{diag}(A)u, v\rangle, \quad \langle u, v\rangle_1 = \langle Au, v\rangle, \quad \langle u, v\rangle_2 = \langle \mathrm{diag}(A)^{-1}Au, Av\rangle. \tag{3}$$

Here $\langle\cdot,\cdot\rangle$ is the Euclidean inner product. Their respective norms are denoted by $\|\cdot\|_i$, $i = 0, 1, 2$.

Throughout this section, we denote the fine and coarse grid levels of the TGM as the h- and H-levels respectively. For smoothing operator, we consider the damped-Jacobi iteration, which is given by

$$G^h = I^{n_h} - \omega \cdot (\mathrm{diag}(A^h))^{-1} A^h \tag{4}$$

see [3, p.10]. The following theorem shows that $\|G^h\|_1 \leq 1$ if ω is properly chosen.

Theorem 1 ([12, p.84]) *Suppose $A > 0$. Let α be such that*

$$\frac{1}{\alpha} \geq \rho(\mathrm{diag}(A)^{-1}A). \tag{5}$$

Then

$$G \equiv I - \alpha \cdot \mathrm{diag}(A)^{-1}A$$

satisfies

$$\|Ge\|_1^2 \leq \|e\|_1^2 - \alpha\|e\|_2^2, \qquad \forall e \in \mathbb{R}^n. \tag{6}$$

Inequality (6) is called the *smoothing condition.* We see from the theorem that the damped-Jacobi method (4) with $\omega = \alpha$ satisfies $\|G\|_1 \leq 1$.

For a Toeplitz matrix A generated by an even function f, we see from (1) that $\rho(A) \leq \max_{\theta\in[-\pi,\pi]} f(\theta)$. Moreover, $\mathrm{diag}(A)$ is just a constant multiple of the identity matrix. Thus it is easy to find an α that satisfies (5). In applications where f is not known a priori, we can estimate a bound of $\rho(A)$ by the Frobenius norm or matrix ∞-norm of A. The estimate can be computed in $O(n)$ operations.

For TGM, the correction operator is given by

$$T^h = I^{n_h} - I_H^h (A^H)^{-1} I_h^H A^h$$

with the convergence factor given by $\|(G^h)^{\nu_2}T^h(G^h)^{\nu_1}\|_1$, see [12, p.89]. Here ν_1 and ν_2 are the numbers of pre- and post-smoothing steps in the MGM algorithm in §2. For simplicity, we will consider only $\nu_2 = 1$ and $\nu_1 = 0$. The other cases can be established similarly as we have $\|G^h\|_1 \le 1$. Thus the convergence factor of our TGM is given by $\|G^hT^h\|_1$. The following theorem gives a general estimate on this quantity.

Theorem 2 ([12, p.89]) *Let $A = A^h > 0$ and let $\alpha > 0$ be chosen such that G^h satisfies the smoothing condition (6), i.e.*

$$\|G^he^h\|_1^2 \le \|e^h\|_1^2 - \alpha\|e^h\|_2^2, \qquad \forall e^h \in \mathbb{R}^{n_h}.$$

Suppose that the interpolation operator I_H^h has full rank and that there exists a scalar $\beta > 0$ such that

$$\min_{e^H \in \mathbb{R}^{n_H}} \|e^h - I_H^h e^H\|_0^2 \le \beta\|e^h\|_1^2, \qquad \forall e^h \in \mathbb{R}^{n_h}. \tag{7}$$

Then $\beta \ge \alpha$ and the convergence factor of the h-H two-level TGM satisfies

$$\|G^hT^h\|_1 \le \sqrt{1 - \frac{\alpha}{\beta}}. \tag{8}$$

Inequality (7) is called the *correcting condition*. From Theorems 1 and 2, we see that if α is chosen according to (5) and that the damped-Jacobi method is used as the smoother, then we only have to establish (7) in order to get the convergence results. We start with the following class of matrices.

3.1 Weakly Diagonally Dominant Toeplitz Matrices

In the following, we write n-by-n Toeplitz matrix A generated by f as $A = \mathcal{T}_n[f]$ and its j-th diagonal as a_j, i.e. $[A]_{0,j} = a_j$ is the j-th Fourier coefficient of f. Let $\mathbb{D}$ be the class of Toeplitz matrices generated by functions f that are even, nonnegative and satisfy

$$a_0 \ge 2\sum_{j=1}^{\infty} |a_j|. \tag{9}$$

Given a matrix $A \in \mathbb{D}$, let l be the first non-zero index such that $a_l \ne 0$. If $a_l < 0$, we define the n_h-by-n_H interpolation operator as

$$I_H^h = \begin{pmatrix} \frac{1}{2}I^l & & \\ I^l & & \\ \frac{1}{2}I^l & \frac{1}{2}I^l & \\ & I^l & \ddots \\ & \frac{1}{2}I^l & \ddots \\ & & \ddots \end{pmatrix}. \tag{10}$$

Here I^l is the l-by-l identity matrix. If $a_l > 0$, we define the interpolation operator as

$$I_H^h = \begin{pmatrix} -\frac{1}{2}I^l & & \\ I^l & & \\ -\frac{1}{2}I^l & -\frac{1}{2}I^l & \\ & I^l & \ddots \\ & -\frac{1}{2}I^l & \ddots \\ & & \ddots \end{pmatrix}. \tag{11}$$

Theorem 3 *Let $A \in \mathbb{D}$ and l be the first non-zero index where $a_l \neq 0$. Let the interpolation operator be chosen as in (10) or (11) according to the sign of a_l. Then there exists a scalar $\beta > 0$ independent of n such that (7) holds. In particular, the convergence factor of TGM is bounded uniformly below 1 independent of n.*

Proof: We will prove the theorem for the case $a_l < 0$. The proof for the case $a_l > 0$ is similar and is sketched at the end of this proof. We first assume that $n_h = (2k+1)l$ for some k. Then according to (10), we have $n_H = kl$. For any $e^h = (e_1, e_2, \cdots, e_{n_h})^t \in \mathbb{R}^{n_h}$, we define

$$e^H = (\tilde{e}_1, \tilde{e}_2, \cdots, \tilde{e}_{n_H})^t \in \mathbb{R}^{n_H},$$

where

$$\tilde{e}_{il+j} = e_{(2i+1)l+j}, \qquad 0 \le i \le k-1, \quad 1 \le j \le l.$$

For ease of indexing, we set $e_i = 0$ for $i \le 0$ and $i > n_h$.

We note that with I_H^h as defined in (10) and the norm $\|\cdot\|_0$ in (3), we have

$$\|e^h - I_H^h e^H\|_0^2 \le a_0 \sum_{i=0}^{k-1} \sum_{j=1}^{l} \{e_{2il+j} - \frac{1}{2}e_{(2i+1)l+j} - \frac{1}{2}e_{(2i-1)l+j}\}^2.$$

Thus (7) is proved if we can bound the right hand side above by $\beta\langle e^h, Ae^h\rangle$ for some β independent of e^h. To do so, we observe that for the right hand side above, we have

$$\begin{aligned} & a_0 \sum_{i=0}^{k-1} \sum_{j=1}^{l} \{e_{2il+j} - \frac{1}{2}e_{(2i+1)l+j} - \frac{1}{2}e_{(2i-1)l+j}\}^2 \\ = \; & a_0 \sum_{i=0}^{k-1} \sum_{j=1}^{l} \{e_{2il+j}^2 + \frac{1}{4}e_{(2i+1)l+j}^2 + \frac{1}{4}e_{(2i-1)l+j}^2 - e_{2il+j}e_{(2i+1)l+j} \\ & \qquad - e_{2il+j}e_{(2i-1)l+j} + \frac{1}{2}e_{(2i+1)l+j}e_{(2i-1)l+j}\} \\ \le \; & a_0 \sum_{i=0}^{k-1} \sum_{j=1}^{l} \{e_{2il+j}^2 + \frac{1}{4}e_{(2i+1)l+j}^2 + \frac{1}{4}e_{(2i-1)l+j}^2 - e_{2il+j}e_{(2i+1)l+j} \\ & \qquad - e_{2il+j}e_{(2i-1)l+j} + \frac{1}{4}e_{(2i+1)l+j}^2 + \frac{1}{4}e_{(2i-1)l+j}^2\} \end{aligned}$$

$$\begin{aligned}
&\leq a_0 \sum_{i=0}^{k-1}\sum_{j=1}^{l}\{e_{2il+j}^2 + \frac{1}{2}e_{(2i+1)l+j}^2 + \frac{1}{2}e_{(2i-1)l+j}^2 - e_{2il+j}e_{(2i+1)l+j} - e_{2il+j}e_{(2i-1)l+j}\} \\
&= a_0 \sum_{m=1}^{n_h}(e_m^2 - e_m e_{m+l}) = a_0\langle e^h, \mathcal{T}_{n_h}[1-\cos l\theta]e^h\rangle
\end{aligned}$$

where $\mathcal{T}_{n_h}[1-\cos l\theta]$ is the n_h-by-n_h Toeplitz matrix generated by $1-\cos l\theta$. Thus

$$\min_{e^H\in\mathbb{R}^{n_H}} \|e^h - I_H^h e^H\|_0^2 \leq a_0\langle e^h, \mathcal{T}_{n_h}[1-\cos l\theta]e^h\rangle, \qquad \forall e^h \in \mathbb{R}^{n_h}. \tag{12}$$

Hence to establish (7), we only have to prove that

$$\langle e^h, \mathcal{T}_{n_h}[1-\cos l\theta]e^h\rangle \leq \beta\langle e^h, Ae^h\rangle, \qquad \forall e^h \in \mathbb{R}^{n_h} \tag{13}$$

for some β independent of e^h. To this end, we note that the n_h-by-n_h matrix A is generated by

$$f_{n_h}(\theta) = a_0 + 2\sum_{j=1}^{n_h-1} a_j \cos j\theta.$$

But by (9),

$$f_{n_h}(\theta) = -2a_l(1-\cos l\theta) + (a_0 + 2a_l) + 2\sum_{\substack{j=1\\ j\neq l}}^{n_h-1} a_j\cos j\theta \geq -2a_l(1-\cos l\theta).$$

In particular, by (1)

$$A + 2a_l\mathcal{T}_{n_h}[1-\cos l\theta] = \mathcal{T}_{n_h}[f_{n_h}(\theta)] + 2a_l\mathcal{T}_{n_h}[1-\cos l\theta] = \mathcal{T}_{n_h}[f_{n_h}(\theta) + 2a_l(1-\cos l\theta)] \geq 0. \tag{14}$$

Thus, by (12), we then have

$$-\frac{a_0}{2a_l}\|e^h\|_1^2 = -\frac{a_0}{2a_l}\langle e^h, Ae^h\rangle \geq a_0\langle e^h, \mathcal{T}_{n_h}[1-\cos l\theta]e^h\rangle \geq \min_{e^H\in\mathbb{R}^{n_H}} \|e^h - I_H^h e^H\|_0^2. \tag{15}$$

Hence (7) holds with

$$\beta = \frac{a_0}{2|a_l|} > 0. \tag{16}$$

Next we consider the case where n_h is not of the form $(2k+1)l$. In this case, we let $k = \lfloor n_h/(2l)\rfloor$, $n_{\tilde{h}} = (2k+1)l > n_h$ and $n_{\tilde{H}} = kl > n_H$. We then embed the vectors e^h and e^H into longer vectors $e^{\tilde{h}}$ and $e^{\tilde{H}}$ of size $n_{\tilde{h}}$ and $n_{\tilde{H}}$ by zeros. Then since

$$\|e^h - I_H^h e^H\|_0^2 \leq \|e^{\tilde{h}} - I_{\tilde{H}}^{\tilde{h}} e^{\tilde{H}}\|_0^2$$

and

$$\langle e^{\tilde{h}}, \mathcal{T}_{n_{\tilde{h}}}[1-\cos l\theta]e^{\tilde{h}}\rangle = \langle e^h, \mathcal{T}_{n_h}[1-\cos l\theta]e^h\rangle$$

we see that the conclusion still holds.

We remark that the case where $a_l > 0$ can be proved similarly. We only have to replace the function $(1-\cos l\theta)$ above by $(1+\cos l\theta)$. Since in this case, $f_{n_h}(\theta) \geq 2a_l(1+\cos l\theta)$, we then have

$$A - 2a_l\mathcal{T}_{n_h}[1+\cos l\theta] = \mathcal{T}_{n_h}[f_{n_h}(\theta) - 2a_l(1+\cos l\theta)] \geq 0. \tag{17}$$

From this, we get (15) and hence (7) with β defined as in (16). $\square$

3.2 More General Toeplitz Matrices

The condition on $\mathbb{D}$ class matrices is too strong. For example, it excludes the matrix $A = \mathcal{T}_n[\theta^2]$. However, from (12) and (13), we see that (7) can be proved if we can find a positive number β independent of n and an integer l such that

$$\beta A \geq a_0 \mathcal{T}_n[1 + \cos l\theta] \qquad \text{or} \qquad \beta A \geq a_0 \mathcal{T}_n[1 - \cos l\theta]. \tag{18}$$

Since by (14) and (17), we see that (18) holds for any matrices B in $\mathbb{D}$, we immediately have the following corollary.

Corollary 1 *Let A be a symmetric positive definite Toeplitz matrix. If there exists a matrix $B \in \mathbb{D}$ such that $A \geq B$. Then (7) holds provided that the interpolation operator for A is chosen to be the same as that for B.*

More generally, we see by (1) that if the generating function f of A satisfies

$$\min_{\theta \in [-\pi, \pi]} \frac{f(\theta)}{1 \pm \cos l\theta} > 0, \tag{19}$$

for some l, then (18) holds. Thus we have the following theorem.

Theorem 4 *Let A be generated by an even function f that satisfies (19) for some l. Let the interpolation operator be chosen as in (10) or (11) according to the sign of a_l. Then (7) holds. In particular, the convergence factor of TGM is uniformly bounded below 1 independent of the matrix size.*

It is easy to prove that (19) holds for any even, nonnegative functions with zeros that are of order 2 or less. As an example, consider $A = \mathcal{T}_n[\theta^2] \notin \mathbb{D}$. Since

$$\theta^2 \geq 4 \sin^2 \left(\frac{\theta}{2} \right) = 2(1 - \cos \theta) \tag{20}$$

and $\mathcal{T}_n[1 - \cos\theta] \in \mathbb{D}$, it follows from Theorem 4 that if the interpolation operator for A is chosen to be the same as that for $\mathcal{T}_n[1 - \cos\theta]$, the convergence factor of the resulting TGM will be bounded uniformly below 1. We note that $\mathcal{T}_n[1 - \cos\theta]$ is just the 1-dimensional discrete Laplacian: $\text{diag}[-1, 2, 1]$. Our interpolation operator here is the same as the usual linear interpolation operator used for such matrices, see [3, p.38]. However, we remark that the matrix $A = \mathcal{T}_n[\theta^2]$ is a dense matrix.

As another example, consider the dense matrix $\mathcal{T}_n[|\theta|]$. Since $\pi|\theta| \geq \theta^2$ on $[-\pi, \pi]$, we have by (20)

$$\mathcal{T}_n[|\theta|] \geq \frac{1}{\pi} \mathcal{T}_n[\theta^2] \geq \frac{2}{\pi} \mathcal{T}_n[1 - \cos\theta].$$

Hence $\mathcal{T}_n[|\theta|]$ can also be handled by TGM with the same linear interpolation operator used for $\mathcal{T}_n[1 - \cos\theta]$.

4 Convergence Results for Full Multigrid Method

In TGM, the matrix A^H on the coarse grid is inverted exactly. From the computational point of view, it will be too expensive. Usually, A^H is not solved exactly, but is approximated using the TGM idea recursively on each coarser grid until we get to the coarsest grid. There the operator is inverted exactly. The resulting algorithm is the full multigrid method (MGM). In §3, we have proved the convergence of TGM for the first level. To establish convergence of MGM, we need to prove the convergence of TGM on coarser levels.

Recall that on the coarser grid, the operator A^H is defined by the Galerkin algorithm (2), i.e. $A^H = I_h^H A^h I_H^h$. We note that if $n_h = (2k+1)l$ for some k, then A^H will be a block-Toeplitz-Toeplitz-block matrix and the blocks are l-by-l Toeplitz matrices. In particular, if $l = 1$, then A^H is still a Toeplitz matrix. However, if n_h is not of the form $(2k+1)l$, then A^H will be a sum of a block-Toeplitz-Toeplitz-block matrix and a low rank matrix (with rank less than or equal to $2l$).

We will only consider the case where $n_h = (2^j - 1)l$ for some j. For then on each level $1 \le m \le q$, $n_m = (2k_m + 1)l$ for some integer k_m. Hence the main diagonals of the coarse-grid operators A^m, $1 \le m \le q$, will still be constant. Recall that from the proof of Theorem 3 that (18) implies (7). We now prove that if (18) holds on a finer level, it holds on the next coarser level when the same interpolation operator is used.

Theorem 5 *Let a_0^h and a_0^H be the main diagonal entries of A^h and A^H respectively. Let the interpolation operator I_H^h be defined as in (10) or (11). Suppose that*

$$A^h \ge \frac{a_0^h}{\beta^h} \mathcal{T}_{n_h}[1 \pm \cos l\theta], \tag{21}$$

for some $\beta^h > 0$ independent of n. Then

$$A^H \ge \frac{a_0^H}{\beta^H} \mathcal{T}_{n_H}[1 - \cos l\theta] \tag{22}$$

with

$$\beta^H = 2\frac{a_0^H \beta^h}{a_0^h}. \tag{23}$$

Proof: We first note that if we define the $(n_H + l)$-by-n_H matrix

$$K \equiv \frac{1}{2}\begin{pmatrix} I^l & I^l & & \\ & I^l & I^l & \\ & & \ddots & \ddots \end{pmatrix}, \tag{24}$$

then there exists a permutation matrix P such that

$$I_H^h = P\begin{pmatrix} I^{n_H} \\ \pm K \end{pmatrix}, \tag{25}$$

(cf (10) and (11)). Moreover, for the same permutation matrix P, we have

$$\mathcal{T}_{n_h}[1 \pm \cos l\theta] = P\begin{pmatrix} I^{n_H} & \mp K^t \\ \mp K & I^{n_H + l} \end{pmatrix} P. \tag{26}$$

By (2) and (21), we have

$$A^H = I_h^H A^h I_H^h \geq \frac{a_0^h}{\beta^h} I_h^H \mathcal{T}_{n_h}[1 \pm \cos l\theta] I_H^h. \tag{27}$$

But by (25) and (26), we have

$$\frac{a_0^h}{\beta^h} I_h^H \mathcal{T}_{n_h}[1 \pm \cos l\theta] I_H^h = \frac{a_0^h}{\beta^h}(I^{n_H}, \pm K^t) \begin{pmatrix} I^{n_H} & \mp K^t \\ \mp K & I^{n_H+l} \end{pmatrix} \begin{pmatrix} I^{n_H} \\ \pm K \end{pmatrix} = \frac{a_0^h}{\beta^h}(I^{n_H} - K^t K) \tag{28}$$

By the definition of K in (24), we have

$$\frac{a_0^h}{\beta^h}(I^{n_H} - K^t K) = \frac{a_0^h}{2\beta^h}\mathcal{T}_{n_H}[1 - \cos l\theta].$$

Combining this with (28), we get

$$\frac{a_0^h}{\beta^h} I_h^H \mathcal{T}_{n_h}[1 \pm \cos l\theta] I_H^h = \frac{a_0^h}{2\beta^h}\mathcal{T}_{n_H}[1 - \cos l\theta]. \tag{29}$$

Hence (27) implies (22) with (23). $\square$

Recall by (5) that we can choose α^h such that

$$\alpha^h A^h \leq a_0^h I^{n_h}.$$

Notice that $K^t K \leq I^{n_h}$ and therefore

$$\alpha^h A^H = \alpha^h I_h^H A^h I_H^h \leq a_0^h I_h^H I_H^h = a_0^h(I^{n_H} + K^t K) \leq 2a_0^h I^{n_H}.$$

Thus on the coarser level, we can choose α^H as

$$\alpha^H = \frac{\alpha^h a_0^H}{2a_0^h}. \tag{30}$$

According to (8), (30) and (23), we see that

$$\|G^H T^H\|_1 \leq \sqrt{1 - \frac{\alpha^H}{\beta^H}} = \sqrt{1 - \frac{\alpha^h a_0^H/(2a_0^h)}{2a_0^H \beta^h / a_0^h}} = \sqrt{1 - \frac{\alpha^h}{4\beta^h}}.$$

Recursively, we can extend this result from the next coarser-level to the q-th level and hence obtain the level-dependent convergence of the MGM:

$$\|G^q T^q\|_1 \leq \sqrt{1 - \frac{\alpha^q}{\beta^q}} = \sqrt{1 - \frac{\alpha^h}{4^{q-1}\beta^h}}.$$

We remark that this level-dependent result is the same as that of most MGM, see for instance [12, 2]. One standard way to overcome level-dependent convergence is to use "better" cycles such as the F- or W-cycles, see [12]. We note however that our numerical results in §6 shows that MGM with V-cycles already gives level-independent convergence.

We remark that we can prove the level-independent convergence of MGM in a special case.

Theorem 6 *Let $f(\theta)$ be such that*

$$c_2(1 \pm \cos l\theta) \geq f(\theta) \geq c_1(1 \pm \cos l\theta), \tag{31}$$

for some integer l and positive constants c_1 and c_2. Then for any $1 \leq m \leq q$,

$$\|G^m T^m\|_1 \leq \sqrt{1 - \frac{c_1}{2c_2}}.$$

Proof: From (31), we have

$$c_2 \mathcal{T}_n[1 \pm \cos l\theta] \geq A \geq c_1 \mathcal{T}_n[1 \pm \cos l\theta].$$

Recalling the Galerkin algorithm (2) and using (29) recursively, we then have

$$\frac{c_2}{2^{m-1}} \mathcal{T}_{n_m}[1 - \cos l\theta] \geq A^m \geq \frac{c_1}{2^{m-1}} \mathcal{T}_{n_m}[1 - \cos l\theta]. \tag{32}$$

By the right-hand inequality and (18), we see that

$$\beta^m = \frac{2^{m-1}}{c_1 a_0^m}.$$

Since $2 \geq (1 \pm \cos l\theta)$ for all θ, we have

$$\frac{c_2}{2^{m-2}} I^{n_m} \geq \frac{c_2}{2^{m-1}} \mathcal{T}_{n_m}(1 \pm \cos l\theta)$$

and hence by the left hand side of (32)

$$\frac{c_2}{2^{m-2}} I^{n_m} \geq A^m.$$

Therefore by the definition of α in (5), we see that

$$\alpha^m = \frac{2^{m-2}}{c_2 a_0^m}.$$

According to (8), we then conclude that

$$\|G^m T^m\|_1 \leq \sqrt{1 - \frac{\alpha^m}{\beta^m}} = \sqrt{1 - \frac{c_1}{2c_2}}. \qquad \square$$

As an example, we see that MGM can be applied to $\mathcal{T}_n[\theta^2]$ with the usual linear interpolation operator and the resulting method will be level-independent. To illustrate how the method works, we now display the sequence of projected matrices in each coarser level for $A_{16} = \mathcal{T}_{16}[\theta^2]$. Since $a_1 = -2 < 0$ for this example, we use the interpolation operator in (10) with $l = 1$. Then $A^m = U^m + L^m$, where U^m are Toeplitz matrices and L^m are rank 1 matrices of the form

$$L^m = \begin{pmatrix} \mathbf{0} & (c^m)^* \\ c^m & \delta^m \end{pmatrix},$$

with c^m being row vectors and δ^m being scalars. Let u^m be the first row of the Toeplitz matrix U^m. Then the sequence of vectors in 3 different levels are given approximately by

$$\begin{aligned}
u^1 &= (\pi^2/3, -2/1^2, 2/2^2, -2/3^2, 2/4^2, -2/5^2, \cdots, -2/15^2),\\
c^1 &= (0, \cdots, 0),\\
\delta^1 &= 0;\\
u^2 &= (1.18, -0.62, 0.02, 0.001, 0.0002, 0.00006, 0.00002, -0.00005),\\
c^2 &= (0, -0.0001, -0.0002, -0.0005, -0.0013, -0.0051, -0.0451),\\
\delta^2 &= 0.9275;\\
u^3 &= (0.5523, -0.2844, 0.0081, 0.0001),\\
c^3 &= (-0.0002, -0.0013, -0.035),\\
\delta^3 &= 1.1926.
\end{aligned}$$

5 Computational Cost

Let us first consider the case where $n = (2^j - 1)l$ for some j. Then on each level, $n_h = (2k+1)l$ for some k. From the MGM algorithm in §2, we see that if we are using the damped-Jacobi method (4), the pre-smoothing and post-smoothing steps become

$$u^m := (I^{n_m} - \omega \cdot \mathrm{diag}(A^m)^{-1} A^m) u^m + \omega \cdot \mathrm{diag}(A^m)^{-1} b^m.$$

Thus the main cost on each level depends on the matrix-vector multiplication $A^m y$ for some vector y. If we are using one pre-smoothing step and one post-smoothing step, then we require two such matrix vector multiplications – one from the post-smoothing and one from the computation of the residual. We do not need the multiplication in the pre-smoothing step since the initial guess u^m is the zero vector.

On the finest level, A is a Toeplitz matrix. Hence Ay can be computed in two $2n$-length FFTs, see for instance [13]. If $l = 1$, then on each coarser level, A^m will still be a Toeplitz matrix. Hence $A^m y$ can be computed in two $2n_m$-length FFTs. When $l > 1$, then on the coarser levels, A^m will be a block-Toeplitz-Toeplitz-block matrix with l-by-l Toeplitz sub-blocks. Therefore $A^m y$ can also be computed in roughly the same amount of time by using 2-dimensional FFTs. Thus the total cost per MGM iteration is about eight $2n$-length FFTs.

In comparison, the circulant-preconditioned conjugate gradient methods require two $2n$-length FFTs and two n-length FFTs per iteration for the multiplication of Ay and $C^{-1}y$ respectively. Here C is the circulant preconditioner, see [13]. The cost can be further reduced to only two $2n$-length FFTs if we first diagonalize the circulant preconditioner. The band-Toeplitz preconditioned conjugate gradient methods require two $2n$-length FFTs and one band-solver where the band-width depends on the order of the zeros, see [4]. Thus the cost per iteration of using MGM is about 4 times as that required by the circulant preconditioned conjugate gradient methods or the band-Toeplitz preconditioned conjugate gradient methods.

Next we consider the case when n is not of the form $(2^j - 1)l$. In that case, on the coarser level, A^m will no longer be a block-Toeplitz-Toeplitz-block matrix. Instead it will be a sum of such a matrix and a low rank matrix (with rank less than $2l$). Thus the cost of multiplying $A^m y$ will be increased by $O(ln)$.

6 Numerical Results

In this section, we apply the MGM algorithm in §2 to ill-conditioned real symmetric Toeplitz systems $A_n u = b$. We choose as solution a random vector u such that $0 \le u_i \le 1$. The right hand side vector b is obtained accordingly. As smoother, we use the damped-Jacobi method (4) with ω chosen as $a_0/\max f(\theta)$ for pre-smoother and $\omega = 2a_0/\max f(\theta)$ for post-smoother. We use one pre-smoothing and one post-smoothing on each level. When the coarse grid size is less than 5, we solve the coarse grid system exactly.

The zero vector is used as the initial guess and the stopping criterion is $\|r_j\|_\infty/\|r_0\|_\infty \le 10^{-7}$, where r_j is the residual vector after j iterations. In the following tables, we give the number of iterations required for convergence using our method, see column under M. For comparison, we also give the number of iterations required by the preconditioned conjugate gradient method with no preconditioner (I), the Strang (S) circulant preconditioner, the T. Chan (C) circulant preconditioner and also the band (B) preconditioners, see [6, 7, 4]. The double asterisk ** signifies more than 200 iterations are needed.

For the first example, we consider functions with single zero at the point $\theta = 0$. The functions we tried are $f(\theta) = 6 - 4\cos\theta - 2\cos 2\theta$ and $f(\theta) = \theta^2$. We note that $\mathcal{T}_n[6 - 4\cos\theta - 2\cos 2\theta] \in \mathbb{D}$ whereas $\mathcal{T}_n[\theta^2] \notin \mathbb{D}$. However, we have $\theta^2 \ge 2 - 2\cos\theta$ and $\mathcal{T}_n[2 - 2\cos\theta] \in \mathbb{D}$. Therefore, according to Corollary 1, we can use the interpolation operator (10) with $l = 1$ for $\mathcal{T}_n[\theta^2]$.

$f(\theta)$	$6 - 4\cos\theta - 2\cos 2\theta$					θ^2				
n	I	S	C	B	M	I	S	C	B	M
64	64	**	14	12	7	78	9	15	10	10
128	128	**	16	12	7	173	9	19	10	10
256	**	**	21	12	7	**	9	25	10	10
512	**	**	27	12	7	**	9	32	10	10
1024	**	**	36	12	7	**	10	42	10	10
2048	**	**	47	12	7	**	10	58	10	10

Table 1: Iteration numbers for functions with single zero of even order.

Next we consider a family of functions with jumps and a single zero at the point $\theta = 0$:

$$J_\alpha(\theta) = \begin{cases} |\theta|^\alpha & \text{if } |\theta| \le \pi/2, \\ 1 & \text{if } |\theta| > \pi/2, \end{cases}$$

where $1 < \alpha < 2$ is a parameter. Since the zero is not of even order, band-Toeplitz preconditioners cannot be constructed. We note that matrices $\mathcal{T}_n[J_\alpha(\theta)]$ are not in $\mathbb{D}$. However, since $J_\alpha(\theta) \ge (1 - \cos\theta)/(2\pi)$ for all θ when $1 < \alpha < 2$, we can still use the interpolation operator defined by $1 - \cos\theta$ for the $\mathcal{T}_n[J_\alpha(\theta)]$. We note that the Fourier coefficients a_j of $J_\alpha(\theta)$ are given by

$$a_j = \frac{2}{\pi}\left(\int_0^{\pi/2} \theta^\alpha \cos j\theta d\theta + \int_{\pi/2}^{\pi} \cos j\theta d\theta\right) = \frac{2}{\pi}\left(\frac{1}{j^{\alpha+1}} \sum_{k=1}^{j} \int_{\frac{(k-1)\pi}{2}}^{\frac{k\pi}{2}} \theta^\alpha \cos\theta d\theta - \frac{\sin\frac{j\pi}{2}}{j}\right),$$

for $j = 1, 2, \cdots$. Since the integrand $\theta^\alpha \cos\theta$ is very smooth in the interval $[(k-1)\pi/2, k\pi/2]$, we have used Simpson's rule with 1001 quadrature points to compute the integrals for each interval. The following table of iteration numbers clearly show the advantage of using multigrid methods over the circulant preconditioned conjugate gradient methods.

$J_\alpha(\theta)$	$\alpha = 1.5$				$\alpha = 1.7$				$\alpha = 1.9$			
n	I	S	C	M	I	S	C	M	I	S	C	M
64	35	9	11	6	36	11	12	6	38	13	13	6
128	64	10	12	6	73	12	13	6	78	16	16	7
256	112	11	13	6	142	15	16	6	163	22	18	7
512	194	13	16	6	**	19	19	6	**	24	23	7
1024	**	15	17	6	**	23	22	6	**	38	30	7
2048	**	16	21	6	**	25	27	6	**	50	39	7
4096	**	22	23	7	**	41	33	7	**	78	50	7
8192	**	25	27	7	**	51	40	7	**	140	67	7

Table 2: Iteration numbers for functions with jump and a zero of fractional order.

Finally, we consider two functions with multiple zeros. They are $f(\theta) = 6 - 4\cos 2\theta - 2\cos 4\theta$ and $f(\theta) = \theta^2(\pi^2 - \theta^2)^2$ with $\mathcal{T}_n[6 - 4\cos 2\theta - 2\cos 4\theta] \in \mathbb{D}$ and $\mathcal{T}_n[\theta^2(\pi^2 - \theta^2)^2] \notin \mathbb{D}$. But we note that $\theta^2(\pi^2 - \theta^2) \geq 1 - \cos 2\theta$ for all θ. Thus both matrices can use the interpolation operator in (10) with $l = 2$. In particular, our interpolation operator will be different from that proposed in [8], which in this case will use the interpolation operator in (10) with $l = 1$. Their resulting MGM converges very slowly with convergence factor very close to 1 (about 0.98 for both functions when $n = 64$). For comparison, we list in Table 3, the number of MGM iterations required by such interpolation operator under column F.

$f(\theta)$	$\theta^2(\pi^2 - \theta^2)^2$						$6 - 4\cos 2\theta - 2\cos 4\theta$					
n	I	S	C	B	M	F	I	S	C	B	M	F
64	60	9	16	13	7	**	23	**	10	11	7	**
128	119	10	20	13	7	**	43	**	12	12	7	**
256	**	13	26	14	7	**	83	**	15	12	7	**
512	**	15	34	14	7	**	162	**	20	12	7	**
1024	**	17	46	15	7	**	**	**	24	12	7	**

Table 3: Iteration numbers for functions with multiple zeros.

7 Concluding Remarks

We have shown that MGM can be used to solve a class of ill-conditioned Toeplitz matrices. The resulting convergence rate is linear. The interpolation operator depends on the location of the first non-zero diagonals of the matrices and its sign.

Here we have only proved the convergence of multigrid method with damped-Jacobi as smoothing operator. However, our numerical results show that multigrid method with some other smoothing operators, such as the red-black Jacobi, block-Jacobi and Gauss-Seidel methods, will give better convergence rate. As an example, for the function $f(\theta) = \theta^2(\pi^2 - \theta^2)$, the convergence factors of MGM with the point- and block-Jacobi methods as smoothing operator are found to be about 0.71 and 0.32 respectively for $64 \leq n \leq 1024$.

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