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Multigrid methods for general Block Toeplitz matrices

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SUMMARY

In this paper we discuss multigrid methods for symmetric positive definite Block Toeplitz matrices. Our Block Toeplitz systems are general in the sense that the individual blocks are not necessarily Toeplitz. We investigate how transfer operators for prolongation and restriction have to be chosen such that our multigrid algorithms converge quickly. We will point out why these transfer operators can be understood as block matrices as well. We explain how our new algorithms can also be combined efficiently with the use of a natural coarse grid operator. Furthermore, we see that our block approach also comes out to be helpful for special Toeplitz matrices. Plenty of numerical experiments confirm that our multigrid solvers lead to optimal order convergence. Copyright © 2000 John Wiley & Sons, Ltd.

KEY WORDS: Multigrid methods, iterative methods, preconditioning, Toeplitz matrices

1. TOEPLITZ MATRICES, GENERATING FUNCTIONS AND MULTIGRID

Let $f(x)$ be a real-valued continuous function on the interval $I = [-\pi, \pi]$ and periodically extended to the whole real axis. On the basis of its Fourier coefficients

$$t_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)e^{-ik\theta}d\theta, \qquad \text{for } k \text{ integer},$$

we can define the sequence of Toeplitz matrices $\{T_n \equiv T_n(f)\}_{n\in\mathbb{N}}$ associated with the generating function $f(x)$. Its entries are given by $(T_n)_{\mu,\nu} = t_{\mu-\nu}$:

$$T_n = \begin{pmatrix} t_0 & t_{-1} & \cdots & \cdots & t_{1-n} \\ t_1 & t_0 & t_{-1} & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & t_1 & t_0 & t_{-1} \\ t_{n-1} & \cdots & \cdots & t_1 & t_0 \end{pmatrix}$$

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Since $f(x)$ is real-valued the matrices T_n are Hermitian. In case $f(x)$ is an even function, we are dealing with a sequence of real symmetric Toeplitz matrices. Furthermore, we know that the spectrum of A_n is contained in $range(f)$.

Example 1: The well-known matrix $tridiag(-0.5, 1, -0.5)$ – which is nothing but a uniform discretization of the one-dimensional Laplacian – is generated by the function $f(x) = -0.5e^{-ix} + 1 - 0.5e^{ix} = 1 - cos(x)$. The eigenvalues of T_n are contained in the interval $[0, 2]$. The small eigenvalues of T_n that lead to the large condition numbers are caused by the zero $x_0 = 0$ of f, $f(x_0) = f(0) = 0$, of multiplicity two.

For more information on Toeplitz matrices and their properties we refer to the book [5] and the overview article [1].

In multigrid methods we need to apply a restriction and prolongation operator: If we use a Galerkin coarse grid operator we can write the coarse grid matrix for a twogrid step as

$$T_{n/2} = E_{n,n/2}^T * B_n^T * T_n * B_n * E_{n,n/2} = P_n^T * T_n * P_n \qquad (1)$$

with a Toeplitz matrix B_n related to a function $b(x)$, and the elementary projection matrix

$$I_{n,n/2} = \begin{pmatrix} 1 & & \\ 0 & 0 & \\ 0 & 1 & 0 \\ & 0 & 0 \\ & 0 & 1 \\ & & . \end{pmatrix} = I(1:n, 1:2:n)$$

in MATLAB-notation with the identity matrix I. As a quick and simple motivation let us make use of the following heuristics: With $\tilde{f}(x) = b(x) * f(x) * b(x)$ the entries of the matrix $B_n^T * T_n * B_n$ in our model are – up to a perturbation of low rank – given by the coefficients of $\tilde{f}(x)$; therefore the coefficients of $T_{n/2}$ can be found by deleting every second entry in $\tilde{f}(x)$:

$$f_2(x) = (1/2) * \left(b^2(\frac{x}{2}) f(\frac{x}{2}) + b^2(\frac{x}{2} + \pi) f(\frac{x}{2} + \pi) \right) . \qquad (2)$$

(Note that the above formula actually comes from a convolution argument and thus – as pointed out e.g. in [3], [4], [10] – it holds in particular also for matrix algebras.)
Let us assume that $f(x)$ has a unique zero x_0 of finite order 2κ in the interval $]-\pi, \pi]$. Now the new matrix $A_{n/2}$ should be closely related to the original A_n. Hence the related function $f_2(x)$ should have a zero with the same multiplicity as $f(x)$. In view of $f(x) \geq 0$ this is only possible if $b(x_0 + \pi) = 0$. Therefore, we can easily motivate to use a prolongation operator of the form

$$b(x) = (cos(x_0) + cos(x))^\kappa . \qquad (3)$$

Multigrid methods for Toeplitz systems were first proposed by Serra and Fiorentino in [3], [4] – and it was them who first came up with (2) and showed that transfer operators corresponding to (3) are suitable. Recently, Serra [9] gave a precise analysis of twogrid optimality suggesting lower and upper bounds for κ in (3). In these papers the focus lies on symmetric positive definite problems generated by functions with a single isolated zero $x_0 \in]-\pi, \pi]$.
In [12] and [2] R. Chan and collaborators also studied multigrid for Toeplitz systems: The work [2] presents solutions for symmetric positive definite Toeplitz problems with entries

$t_1 = \cdots = t_l = 0$, $l < n$, like e.g. the matrices generated by $f(x) = 1 - cos((l+1) * x)$.
All the articles mentioned so far employ Galerkin coarse grid operators: However, in general, this will result in a loss of Toeplitz structure on the coarser levels. In a very recent research paper [8] the authors presented a resort for this difficulty using a natural coarse grid operator, i.e. the coarse level representations are nothing but Toeplitz matrices of smaller size generated by the original function f. There we have pointed out how natural coarse grid operators can be employed efficiently for nonnegative generating functions with a finite number of equidistant zeros in $]-\pi, \pi]$ – and we note that for this approach the systems need to be diagonally scaled in advance such that one of the zeros of highest order is shifted to the origin (see [8], sec. 2 and sec. 3, for details).

2. BLOCK TOEPLITZ MATRICES

In the following we consider symmetric Block Toeplitz matrices

$$A_n = \begin{pmatrix} T_0 & T_{-1} & \cdots & T_{1-n} \\ T_1 & T_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & T_{-1} \\ T_{n-1} & \cdots & T_1 & T_0 \end{pmatrix}$$

with $k \times k$ matrices T_j and we will assume that they are generated by the matrix function

$$F(x) = \cdots + T_{-2}e^{-2ix} + T_{-1}e^{-ix} + T_0 + T_1 e^{ix} + T_2 e^{2ix} + \cdots .$$

We would like to stress that this is the first paper studying multigrid in the case that the individual blocks T_j are not necessarily Toeplitz. In other words: Our investigations are very much different from the studies on multigrid for Block Toeplitz with Toeplitz blocks in [4] or [13] (– where the block size k was variable, but the blocks were Toeplitz).
Example 2: The sparse matrix A_n with

$$T_0 = \begin{pmatrix} 3 & -1 \\ -1 & 2 \end{pmatrix}, \; T_{-1} = \begin{pmatrix} 0 & 0 \\ 1 & 10 \end{pmatrix}$$

is generated by the 2×2 matrix function

$$F(x) = \begin{pmatrix} 3 & -1 + e^{ix} \\ -1 + e^{-ix} & 2 + 20\cos(x) \end{pmatrix} .$$

3. BLOCK TOEPLITZ MATRICES WITH DIAGONAL GENERATING MATRIX FUNCTIONS

First let us consider Block Toeplitz matrices with n diagonal blocks T_j of size $k \times k$. The generating function is then also a diagonal matrix function of the form

$$F(x) = \Lambda(x) = \begin{pmatrix} \lambda_1(x) & 0 & \cdots & 0 \\ 0 & \lambda_2(x) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_k(x) \end{pmatrix} .$$

By a simple permutation which interchanges the order of the indices $T_{j,m}$ we can transform the Block Toeplitz matrix into a diagonal Block matrix with k Toeplitz matrices of size $n \times n$ as diagonal blocks. Let us also assume that $\lambda_m(x)$ has only got a single isolated zero $\tilde{x}_m \in]-\pi, \pi]$: Then for each Toeplitz block we can define a multigrid prolongation according to (3) – just as described in the scalar case – related to the generating function $\lambda_m(x)$. That way for each $\lambda_m(x)$ we introduce a generating function $b_m(x)$ such that for every zero $\tilde{x}_m$ of $\lambda_m(x)$ there holds $b_m(\tilde{x}_m) = 0$. The multigrid method for each block can be seen as a multigrid algorithm for the given Block Toeplitz matrix with prolongation defined by the Block Toeplitz generated by the function

$$B(x) = \begin{pmatrix} b_1(x) & 0 & \cdots & 0 \\ 0 & b_2(x) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & b_k(x) \end{pmatrix} .$$

The elementary projection matrix that has to be applied is given by the block matrix

$$I_{n,n/2,k} = \begin{pmatrix} I_k & & \\ 0_k & 0_k & \\ 0_k & I_k & 0_k \\ & 0_k & 0_k \\ & 0_k & I_k \\ & & . \end{pmatrix} .$$

with I_k and 0_k denoting the $k \times k$ identity and the $k \times k$ matrix of zeros, respectively. (Note that the same kind of transfer operators has previously been suggested by R. Chan and collaborators in [2] for symmetric positive Toeplitz matrices with zero entries below the main diagonal, i.e. for the case $t_1 = \cdots = t_l = 0$, with an integer l smaller than the matrix size.)
Hence multigrid for Block Toeplitz matrices with generating block diagonal function can be reduced to Multigrid for k independent scalar Toeplitz matrices. Then the prolongation/restriction matrix is a sparse Block Toeplitz matrix with diagonal generating matrix function depending on the zeros of the eigenvalue functions $\lambda_m(x)$. We also mention that a natural coarse grid operator – instead of a Galerkin approach – will be applicable if the zeros of all the functions $\lambda_m(x)$, $m = 1, \ldots, k$, are situated at the origin.

4. MULTIGRID FOR GENERAL BLOCK TOEPLITZ SYSTEMS

For motivation let us again start with the case of a Galerkin coarse grid representation: Similar to the scalar case for generating function $F(x)$ and a chosen prolongation/restriction – with generating function $B(x)$ and elementary projection $E_{n,n/2,k}$ – the Galerkin coarse grid matrix of half size

$$A_{n/2} = I_{n,n/2,k}^T * B_n^T * A_n * B_n * I_{n,n/2,k}$$

is "associated" (– i.e. we ignore low rank perturbations for a moment –) to the matrix function

$$F_2(x) = (1/2) * \left(B(\frac{x}{2}) f(\frac{x}{2}) B(\frac{x}{2}) + B(\frac{x}{2} + \pi) f(\frac{x}{2} + \pi) B(\frac{x}{2} + \pi) \right) .$$

In general, we can analyse the properties of F_2 only in the case that F_2 can be transformed to a diagonal matrix. Therefore we choose $B(x) = b(x) * I_k$ and assume that $F(x/2)$ and $F(x/2 + \pi)$ are commuting matrices; then both can be diagonalized by the same eigenvector matrix: $F(x) = U^H(x)D(x)U(x)$ and $F(x+\pi) = U^H(x)D_\pi(x)U(x)$. Under these assumptions we derive that the original problem is related to a multigrid method applied on the Block Toeplitz matrix with **diagonal** generating function

$$\tilde{F}(x) = \Lambda(x) = U(x)F(x)U^H(x) = D(x)$$

with $B(x) = b(x)I_k$ and

$$\tilde{F}_2(x) = b^2(x/2)D(x/2+\pi) + b^2(x/2+\pi)D(x/2) \ .$$

Thereby we have to choose $b(x)$ such that it has zeros at every position where one of the eigenvalue functions $\lambda_m(x)$ is zero. In the following we shall assume that all the eigenvalue functions $\lambda_m(x)$ have only got a single isolated zero and then there will be no problems. (However, note in passing that - just as in the scalar case – rather severe problems might arise if any of the $\lambda_m(x)$ has two isolated zeros in distance π [2],[8].) If, furthermore, all these zeros are at the origin, then we can again completely avoid the algorithmic difficulties associated with the Galerkin coarse grid representation and use a natural coarse grid operator.

5. TOEPLITZ MATRICES CONSIDERED AS BLOCK TOEPLITZ MATRICES

Every Toeplitz matrix of size n can be considered as a Block Toeplitz matrix with blocksize k iff n is an integer multiple of k. Here we restrict ourselves to the simplest and most interesting case $k = 2$. For T_n generated by the function $f(x)$ we can partition T_n in blocks of size 2×2 in the form

$$T_n = \left(\begin{array}{cc|cc|cc|cc}
t_0 & t_{-1} & t_{-2} & t_{-3} & \cdots & \cdots & t_{2-n} & t_{1-n} \\
t_1 & t_0 & t_{-1} & t_{-2} & \cdots & \cdots & t_{3-n} & t_{2-n} \\
\hline
t_2 & t_1 & \ddots & & & & \vdots & \vdots \\
t_3 & t_2 & & \ddots & & & \vdots & \vdots \\
\hline
\vdots & \vdots & & & \ddots & & t_{-2} & t_{-3} \\
\vdots & \vdots & & & & \ddots & t_{-1} & t_{-2} \\
\hline
t_{n-2} & t_{n-3} & \cdots & \cdots & t_2 & t_1 & t_0 & t_{-1} \\
t_{n-1} & t_{n-2} & \cdots & \cdots & t_3 & t_2 & t_1 & t_0
\end{array} \right)$$

and write the generating matrix function as

$$F(x) = \cdots + e^{-ix} \begin{pmatrix} t_2 & t_1 \\ t_3 & t_2 \end{pmatrix} + \begin{pmatrix} t_0 & t_{-1} \\ t_1 & t_0 \end{pmatrix} + e^{ix} \begin{pmatrix} t_{-2} & t_{-3} \\ t_{-1} & t_{-2} \end{pmatrix} + \cdots =$$

$$= \frac{1}{2} \begin{pmatrix} f(x/2) + f(x/2+\pi) & e^{ix/2}(f(x/2) - f(x/2+\pi)) \\ e^{-ix/2}(f(x/2) - f(x/2+\pi)) & f(x/2) + f(x/2+\pi) \end{pmatrix} .$$

The eigenvalues of the matrix $F(x)$ are given by

$$\lambda_0(x) = f(\frac{x}{2}) \quad \text{and} \quad \lambda_1(x) = f(\frac{x}{2} + \pi) \tag{4}$$

If $f(x)$ has exactly two zeros x_0 and $x_1 = x_0 + \pi$, then the eigenvalues $\lambda_0(x)$ and $\lambda_1(x)$ of the generating 2×2 matrix function $F(x)$ have only got one zero at $2x_0 = 2x_1$ (with the orders of the zeros of $\lambda_0(x)$ and $\lambda_1(x)$ corresponding to the orders of the zeros x_0 and x_1 of $f(x)$.) Assuming $f(x)$ has only got zeros of order at most 2 we can certainly choose $B(x) = (cos(x_0) + cos(x)) * I_2$ as restriction/prolongation matrix. (As we already mentioned twice before, the same transfer operators have previously been suggested in the case $x_0 = 0$ for very special Toeplitz problems in [2].) Note also that $F(x)$ and $F(x + \pi)$ are commuting and therefore the results of section 4 are valid, in fact.
It is very well-known e.g. from [2], [8] or [11] that one should most certainly not use the above block approach with $k = 2$ for a Toeplitz problem generated by a function with a single isolated zero $x_0 \in]-\pi, \pi]$ like e.g. $f(x) = 1 - cos(x)$ or $f(x) = x^2$. However, if standard multigrid (i.e. using standard linear interpolation corresponding to $b(x) = 1 + cos(x)$ for prolongation and its transpose for restriction) fails for a sequence of Toeplitz matrices – like e.g. the ones generated by $f(x) = 1 - cos(2x)$ – because of zeros of distance π then our analysis underlines that the block method is the approach that is properly called for and it explains why the corresponding transfer operators lead to fast convergence.

Example 3: We consider the Toeplitz matrix related to the generating function $f(x) = 1 - cos(2x)$ with zeros 0 and π. The generating function for the block matrix is given by

$$F(x) = \begin{pmatrix} 1 - cos(x) & 0 \\ 0 & 1 - cos(x) \end{pmatrix} = (1 - cos(x)) * I_2 \ .$$

By permutation we can transform the related Toeplitz matrix $pentadiag(-1, 0, 2, 0, -1)$ into

$$\begin{pmatrix} tridiag(-1, 2, -1) & 0 \\ 0 & tridiag(-1, 2, -1) \end{pmatrix} .$$

Therefore the standard multigrid algorithm on these two Toeplitz blocks is equivalent to the block Multigrid method on the original matrix with prolongation/restriction given by $B(x) = (1 + cos(x))I_2$.

6. NUMERICAL EXAMPLES

We would now like to test our algorithmic ideas numerically and we would first of all like to explain the general setting of our experiments:
We will only list results for W-cycle multigrid solvers. (For more algorithmic details on multigrid we refer to the books [6], [14].) The coarsest level is fixed in all our tests as an 8×8-matrix. Furthermore, we employ the following stopping criterion to obtain the iteration counts we list in Table 1:

$$\frac{\|r^{(j)}\|_2}{\|r^{(0)}\|_2} \leq 10^{-7}$$

Here $r^{(j)}$ denotes the residual after j iterations and $r^{(0)}$ the original residual, i.e. we stop iterating when the relative residual corresponding to the Euclidian norm is less or equal 10^{-7}.

We always use two steps of the Richardson method for pre- and postsmoothing in our multigrid cycles. Motivated by [3] and [4] we use the damping parameters $\omega_1 = 1/\max_{\theta\in[-\pi,\pi]} \|G(\theta)\|_2$ for presmoothing and $\omega_2 = 2/\max_{\theta\in[-\pi,\pi]} \|G(\theta)\|_2$ for postsmoothing, respectively.

Let us now take a look at two rather challenging sparse examples and start with

$$G_1(x) = \begin{pmatrix} 1+cos(x) & 0 \\ 0 & 1-cos(x) \end{pmatrix}.$$

Since this Block Toeplitz matrix also involves a zero at π, we need to apply a Galerkin coarse grid operator. However, here the loss of structure on the coarser levels does not matter as the example is sparse. Note that in transferring residuals from and to the finest level we need to use prolongations and restrictions corresponding to

$$B_1^{finest}(x) = \begin{pmatrix} 1-cos(x) & 0 \\ 0 & 1+cos(x) \end{pmatrix}.$$

However, as long as only coarse levels are involved, transfer operators based on $B(x) = (1+cos(x))I_2$ should be used. This idea is very strongly related to the so-called "Matrix Multilevel Method" for general sparse matrices proposed in [7]. We observe in Table 1 that iteration numbers are independent of the matrix size .
The matrix function

$$G_2(x) = \begin{pmatrix} 2 & -(1+\frac{1}{2}cos(x)) \\ -(1+\frac{1}{2}cos(x)) & 2 \end{pmatrix}$$

is associated with a single isolated zero of order 2 at the origin – and thus we may use a natural coarse grid operator. Hence, independently of the level, the appropriate transfer operators will be given by $B(x) = (1+cos(x))I_2$. Again, we observe optimal order convergence.
However, giving results for dense problems as well is crucial:

$$G_3(x) = \begin{pmatrix} x^2 & 0 \\ 0 & 1-cos(x) \end{pmatrix}$$

Just as for G_2, we are again dealing with a single isolated zero at the origin: Thus again transfer operators based on $B(x) = (1+cos(x))I_2$ need to be used. We take this chance to compare the performance for using natural and Galerkin coarse grid operators. Note that – although iteration counts in the Galerkin case are slightly smaller – this outlines very clearly why the natural coarse grid operator is superior for this dense problem: In the Galerkin case we lose the matrix structure on the coarse levels. On the other hand, we can make use of this structure algorithmically on every level when using the natural coarse grid operator and, furthermore, we will still get a convergence rate independent of the matrix size and the iteration numbers are almost the same.
Finally, we investigate the Toeplitz problem generated by

$$G_4(x) = x * sin(x),$$

i.e. we have a zero of order 2 at $x_0 = 0$ plus a zero of order 1 at $x_1 = \pi$. We know from section 5 that again transfer operators for prolongation and restriction based on $B(x) = (1+cos(x))I_2$ are the variant of choice. (Note that matrices generated by G_4 have not actually been covered in the paper [2], since we know from the Fourier expansion that we are in general dealing with dense matrices without any zero entries.) Again, we confirm that employing a natural coarse grid operator is strongly preferable to Galerkin coarsening in this case: Here iteration numbers are even the same for both approaches. (For some more reasoning and comparisons concerning natural and Galerkin coarse grid operators in the Toeplitz context see the Ph.D. thesis [11].)

number of unknowns	64	128	256	512	1024	2048	4096	8192	16384
Problem G_1 and "Galerkin"	5	6	6	6	6	6	6	6	6
Problem G_2 and "natural"	13	14	14	15	14	15	15	15	15
Problem G_3 and "Galerkin"	11	11	11	11	11	11	11	11	11
Problem G_3 and "natural"	14	14	14	14	14	14	14	14	14
Problem G_4 and "Galerkin"	10	10	10	10	10	10	10	10	10
Problem G_4 and "natural"	10	10	10	10	10	10	10	10	10

Table 1. Iteration counts for our W-cycle solvers.

We can summarize that our numerical experiments confirm strikingly that our new multigrid algorithms lead to optimal order convergence independent of the matrix size, i.e. for sparse problems the computational complexity for the multigrid solution is of order $O(n)$ whereas for dense problems (and natural coarse grid operators) it is of order $O(n \log n)$.

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