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Abstract

Aim of the paper is to analyze multigrid methods based on smoothed aggregation in the case of circulant and Toeplitz matrices. The analysis is based on the classical convergence theory for these types of matrices and results in optimal smoothing parameters that have to be chosen for the smoothing of the grid transfer operators in order to guarantee optimality of the resulting multigrid method. The theoretical findings are backed up by numerical experiments.

Keywords: multigrid methods, Toeplitz matrices, circulant matrices, smoothed aggregation-based multigrid
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1. Introduction

The development of multigrid methods for τ-matrices and Toeplitz matrices go back to [1], the two level case was considered in [2]. Using the same ideas methods for circulant matrices were developed later in [3, 4]. While these works provide the basis to develop and analyze multigrid methods for Toeplitz matrices and matrices from different matrix algebras, including the τ- and circulant algebra, they did not provide a prove of optimality of the multigrid cycle, in the sense that the convergence rate is bounded by a constant $c < 1$ independent on the number of levels used in the multigrid cycle. This prove was added later in [5, 6].

The theory that is used to build up the two-grid and multigrid methods and to prove their convergence is based on the classical variational multigrid theory, as it is presented in e.g. [7, 8, 9, 10].

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1.1. Toeplitz and circulant matrices

A Toeplitz matrix $T_n \in \mathbb{C}^{n\times n}$ is a matrix with constant entries on the diagonals, i.e. T_n is of the form

$$T_n = \begin{pmatrix} t_0 & t_{-1} & t_{-2} & \cdots & t_{-n+1} \\ t_1 & t_0 & t_{-1} & \ddots & \vdots \\ t_2 & t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ t_{n-1} & t_{n-2} & t_{n-3} & \cdots & t_0 \end{pmatrix}. \tag{1}$$

As a consequence the matrix entries are completely determined by the $2n-1$ values $t_{-n+1}, \dots, t_{n-1}$. There exists a close relationship of a Toeplitz matrix to its generating symbol $f : \mathbb{R} \to \mathbb{C}$, a 2π-periodic function given by

$$f(x) = \sum_{j=-\infty}^{\infty} t_j \mathrm{e}^{\mathrm{i}2\pi jx}, \tag{2}$$

so the entries on the diagonals are given as the Fourier coefficients of f and consequently by

$$t_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \mathrm{e}^{-\mathrm{i}2\pi jx} dx. \tag{3}$$

The generating symbol f always induces a sequence $\{\mathcal{T}_n(f)\}_{n=1}^{\infty}$ of Toeplitz matrices $\mathcal{T}_n(f)$. In the case of f being a trigonometric polynomial, the resulting Toeplitz matrices are band matrices for n large enough. There are various theoretical results on sequences of Toeplitz matrices and their generating symbol, most important for the analysis of iterative methods for Toeplitz matrices is the fact that the distribution of the eigenvalues of the Toeplitz matrix is given by the generating symbol in the limit case $n \to \infty$, for details see [11].

Circulant matrices are of a very similar form. A circulant matrix is a Toeplitz matrix, where the entry $t_{-k} = t_{n-k}$, $k = 1, 2, \dots,$ i.e.

$$C_n = \begin{pmatrix} t_0 & t_{n-1} & t_{n-2} & \cdots & t_1 \\ t_1 & t_0 & t_1 & \ddots & \vdots \\ t_2 & t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ t_{n-1} & t_{n-2} & t_{n-3} & \cdots & t_0 \end{pmatrix}.$$

With the help of the matrix Z_n that is given by

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

C_n can alternatively be written as

$$C_n = \sum_{j=0}^{n-1} t_j Z_n^j,$$

further C_n is diagonalized by the Fourier matrix F_n, where

$$(F_n)_{j,k} = \frac{1}{\sqrt{n}} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{n} jk}, \qquad j,k = 0,\dots,n-1,$$

i.e.

$$C_n = F_n \operatorname{diag}(\lambda^{(n)}) F_n^H,$$

for $\lambda^{(n)} = (\lambda_0^{(n)},\dots,\lambda_{n-1}^{(n)})$ given by

$$\lambda_j^{(n)} = f\left(\frac{2\pi j}{n}\right), \qquad j = 0,\dots,n-1.$$

Allowing negative indices to denote the diagonals above the main diagonal as in the Toeplitz case, i.e. in (1), results in demanding $t_k = t_{k \bmod n}$. Using the generating symbol f in (2) similarly to the Toeplitz case a sequence $\{\mathcal{C}_n(f)\}_{n=1}^\infty$ of matrices $\mathcal{C}_n(f)$ is defined. In contrast to the Toeplitz case the circulant matrices form a matrix algebra as they are diagonalized by the Fourier matrix F_n.

The concept of Toeplitz and circulant matrices can easily be extended to the block case, i.e. the case where the matrix entries are not elements of the field of complex numbers but rather of the ring of $m \times m$ matrices. In this case the generating symbol becomes a matrix-valued 2π-periodic function and the matrices are called block Toeplitz and block circulant matrices, respectively. The aforementioned properties of the matrices transfer to this case, e.g. a block circulant matrix with block size $m \times m$ and n blocks on the main diagonal is block diagonalized by $F_n \otimes I_m$, where $\otimes$ denotes the Kronecker product and I_m denotes the identity matrix of size $m \times m$. The analysis of multigrid methods with more general blocks is beyond the scope of this article, for further details see e.g. [12].

An interesting special type of block matrices that we will deal with is the case where the blocks itself are Toeplitz/circulant, again. The resulting matrix will be called block Toeplitz Toeplitz block (BTTB) or block circulant circulant (BCCB) and it can be described by a bivariate 2π-periodic generating symbol f. In the d-level case the generating symbols are $f : \mathbb{R}^d \to \mathbb{C}$ a 2π periodic functions having Fourier coefficients

$$t_j = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} f(x) \mathrm{e}^{-\mathrm{i}\langle j|x\rangle}\, dx, \qquad j = (j_1,\dots,j_d) \in \mathbb{Z}^d,$$

where $\langle \cdot | \cdot \rangle$ denotes the usual scalar product between vectors. From the coefficients t_j one can build the sequence $\{\mathcal{C}_n(f)\}$, $n = (n_1,\dots,n_d) \in \mathbb{N}^d$, of multilevel circulant matrices of size $N = \prod_{r=1}^{d} n_r$. Every matrix $\mathcal{C}_n(f)$ is explicitly written as

$$\begin{aligned} \mathcal{C}_n(f) &= \sum_{|j| \leqslant n-e} a_j (Z_{n_1}^{j_1} \otimes \cdots \otimes Z_{n_d}^{j_d}) \\ &= \sum_{|j_1| \leqslant n_1 - 1} \cdots \sum_{|j_d| \leqslant n_d - 1} a_{(j_1,\ldots,j_d)} Z_{n_1}^{j_1} \otimes \cdots \otimes Z_{n_d}^{j_d}, \end{aligned}$$

Here $\otimes$ denotes the usual Kronecker product, so that $A \otimes B$ is the block matrix $[a_{ij}B]_{ij}$, $e = (1, \ldots, 1) \in \mathbb{N}^d$ and the relations between two multi-indices (as $|j| \leqslant n - e$) should be intended componentwise. Defining the d-dimensional Fourier matrix $F_n = F_{n_1} \otimes \cdots \otimes F_{n_d}$, the matrix $\mathcal{C}_n(f)$ can be written as

$$\mathcal{C}_n(f) = F_n \operatorname{diag}(\lambda^{(n)}) F_n^H,$$

where $\lambda^{(n)} = \lambda^{(n_1)} \times \cdots \times \lambda^{(n_d)}$ if n is a d-index.

1.2. Multigrid methods

A multigrid method is a method to solve a linear system of equations. When traditional stationary iterative methods like Jacobi are used to solve a linear system, the methods perform poorly when the system gets more ill-conditioned, e.g. when the mesh width is decreased in the discretization of a PDE. The reason for this is that error components belonging to large eigenvalues are damped efficiently, while error components belonging to small eigenvalues get damped slowly. In the discretized PDE example the first correspond to the rough error modes, while the latter correspond to the smooth error modes. For this reason methods like Jacobi are known as “smoothers”. Motivated by the PDE-case the construction of a two-grid method proceeds by computing the residual, resampling it on a coarser grid, where the smooth components are “rougher”, and solving for an approximate error on the coarser grid. This approximation is then used to correct the current approximate solution, this correction can be followed by another application of the smoother. Proceeding in this manner finally yields a multigrid solution where only on the coarsest grid the system is solved directly, applying $\xi = 1, 2, \ldots$ recursive calls yields different cycling strategies.

To construct a multigrid method various components have to be chosen. Assume that the solution of a linear system

$$Ax = b,$$

where $A \in \mathbb{C}^{N \times N}$, $x \in \mathbb{C}^N$ and $b \in \mathbb{C}^N$ is sought for. To construct a multigrid method the system on the finest level is denoted by $A_0 = A$, the multi-index of the size is denoted by $n_0 = n \in \mathbb{N}^d$. The multi-indices of the system sizes on the coarser grids are then denoted by $n_i < n_{i-1}$,

$i = 1, \dots, l_{\max}$, where $l_{\max}$ is the maximum number of levels used. Defining $N_i = \prod_{j=1}^{d} (n_i)_j$, to transfer a quantity from one level to another restriction operators $R_i : \mathbb{C}^{N_i} \to \mathbb{C}^{N_{i+1}}$, $i = 0, \dots, l_{\max} - 1$ and $P_i : \mathbb{C}^{N_{i+1}} \to \mathbb{C}^{N_i}$, $i = 0, \dots, l_{\max} - 1$ are needed, furthermore a hierarchy of operators $A_i \in \mathbb{C}^{N_i \times N_i}$, $i = 1, \dots, l_{\max}$ has to be defined. On each level appropriate smoothers $\mathcal{S}_i$ and $\tilde{\mathcal{S}}_i$ and the numbers of smoothing steps ν_1 and ν_2 have to be chosen, we limit ourselves to stationary iterative methods although other smoother like Krylov-subspace methods can be used, as well. After ν_1 presmoothing steps using $\mathcal{S}_i$, the residual $r_{n_i} \in \mathbb{C}^{N_i}$ is computed and restricted to the coarse grid, the result is $r_{n_{i+1}}$. On the coarse grid the error is computed by solving

$$A_{i+1} e_{n_{i+1}} = r_{n_{i+1}},$$

in the multigrid case this is done by a recursive application of the multigrid method. The resulting error is interpolated back to obtain the fine level error e_i and the current iterate is updated using this error. Afterwards, the iterate is improved by postsmoothing. The process of correcting the current iterate using the coarse level is known as *coarse grid correction*, it has the iteration matrix

$$M_i = I - P_i A_{i+1}^{-1} R_i A_i. \qquad (4)$$

In summary the multigrid method $\mathcal{MG}_i$ is given by Algorithm 1.

Algorithm 1 Multigrid cycle $x_{n_i} = \mathcal{MG}_i(x_{n_i}, b_{n_i})$

$x_{n_i} \leftarrow \mathcal{S}_i^{\nu_1}(x_{n_i}, b_{n_i})$
$r_{n_i} \leftarrow b_{n_i} - A_i x_{n_i}$
$r_{n_{i+1}} \leftarrow R_i r_{n_i}$
$e_{n_{i+1}} \leftarrow 0$
if $i + 1 = l_{\max}$ **then**
  $e_{n_{l_{\max}}} \leftarrow A_{l_{\max}}^{-1} r_{n_{l_{\max}}}$
else
  for $j = 1, \dots, \xi$ **do**
    $e_{n_{i+1}} \leftarrow \mathcal{MG}_{i+1}(e_{n_{i+1}}, r_{n_{i+1}})$
  end for
end if
$e_{n_i} \leftarrow P_i e_{n_{i+1}}$
$x_{n_i} \leftarrow x_{n_i} + e_{n_i}$
$x_{n_i} \leftarrow \tilde{\mathcal{S}}_i^{\nu_2}(x_{n_i}, b_{n_i})$

The classical algebraic convergence analysis is based on two properties, the smoothing property and the approximation property that are coupled together by an appropriately chosen norm $\|\cdot\|_*$, where in the classical AMG theory the $AD^{-1}A$-norm with $D = \operatorname{diag}(A)$ is chosen and in the circulant case the A^2-norm turns out to be helpful. The two properties are given by the following definitions:

Definition 1.1 (Smoothing properties)**.** *An iterative method $\mathcal{S}_i$ with iteration matrix S_i fulfills the* presmoothing property *if there exists an $\alpha > 0$ such that for all $v_{n_i} \in \mathbb{C}^{N_i}$ it holds*

$$\|S_i v_{n_i}\|_{A_i}^2 \leq \|v_{n_i}\|_{A_i}^2 - \alpha \|S_i v_{n_i}\|_*^2. \tag{5}$$

Analogously, it fulfills the postsmoothing property *if there exists a $\beta > 0$ such that*

$$\|S_i v_{n_i}\|_{A_i}^2 \leq \|v_{n_i}\|_{A_i}^2 - \beta \|v_{n_i}\|_*^2. \tag{6}$$

Definition 1.2 (Approximation property)**.** *Let M_i be the iteration matrix of the coarse grid correction defined in* (4)*. The coarse grid correction fulfills the* approximation property *if there exists a γ for all $v_{n_i} \in \mathbb{C}^{N_i}$ such that*

$$\|M_i v_{n_i}\|_{A_i}^2 \leq \gamma \|v_{n_i}\|_*^2. \tag{7}$$

To show convergence of a multigrid method, usually, R_i is chosen to be the adjoint of P_i and the coarse grid operator A_{i+1} is chosen as the Galerkin coarse grid operator $P_i^H A_i P_i$. Using a variational argument it can then be shown that the resulting method converges, for details we refer to [10]. If both smoothing and approximation properties are fulfilled, one easily shows that a two-grid method converges, as stated by the following lemma for the postsmoothing.

Lemma 1.3. *Assume that $R_i = P_i^H$ and $A_{i+1} = P_i^H A_i P_i$, let $\mathcal{S}_i$ be a smoother with iteration matrix S_i fulfilling the postsmoothing property* (6) *for $\beta > 0$ and let the coarse grid correction fulfill the approximation property* (7) *for $\gamma > 0$ with the same norm $\|\cdot\|_*$. Then we have $\gamma \geq \beta$ and for all $v_{n_i} \in \mathbb{C}^{N_i}$*

$$\|S_i M_i v_{n_i}\|_{A_i} \leq \sqrt{1 - \beta/\gamma} \|v_{n_i}\|_{A_i}.$$

The proof of this lemma as well as results regardig two-grid methods using presmoothing or both can be found e.g. in [10].

2. Multigrid for circulant and Toeplitz matrices

In the following, we will introduce multigrid methods for circulant matrices and briefly review the convergence results for these methods, as our analysis of aggregation based methods is based on such results. After that, we will provide an overview over the modifications necessary to deal with Toeplitz matrices in a conceptually very similar way.

Let f_i be the symbol of A_i, in this paper we assume $f_i \geq 0$ thus A_i is positive definite (adding the Strang correction if necessary). In general, to design a multigrid method, the smoother, a coarse level with fewer degrees of freedom and the prolongation and restriction have to be chosen appropriately. The common choice for both, pre- and postsmoothing is relaxed Richardson, i.e. $\mathcal{S}_i$ is chosen as

$$\mathcal{S}_i(x_{n_i}, b_{n_i}) = \underbrace{(I - \omega_i A_i)}_{=S_i} x_{n_i} + \omega_i b_{n_i},$$

and $\tilde{\mathcal{S}}_i$ is chosen like this, but with a different $\tilde{\omega}_i$. Using appropriate relaxation parameters ω_i and $\tilde{\omega}_i$ this smoother fulfills the presmoothing property (5) respectively the postsmoothing property (6) as stated by the following theorem that can be found as Proposition 3 in [6].

Theorem 2.1. *Let $A_i = \mathcal{C}_{n_i}(f_i)$, where $f_i : \mathbb{R}^d \to \mathbb{R}$ and let $\mathcal{S}_i$ as defined above with $\omega_i \in \mathbb{R}$. Then for all $v_{n_i} \in \mathbb{C}^{N_i}$ and $\nu_1 \in \mathbb{N}$*

$$\|S_i^{\nu_1} v_{n_i}\|_A^2 \leq \|v_{n_i}\|_A^2 - \alpha \|S_i^{\nu_1} v_{n_i}\|_{A^2}^2$$

holds, if one of the following two is satisfied:

1. $0 \leq \omega_i \leq 1/\|f_i\|_\infty$ *or*
2. $1/\|f_i\|_\infty < \omega_i \leq 2/\|f_i\|_\infty$.

In the first case we have $\alpha < 2\omega_i \nu_1$, in the latter we obtain

$$\alpha \leq \min \left\{ 2\omega_i \nu_1, \frac{1}{\|f_i\|_\infty} \left[\frac{1}{(1 - \omega_i \|f_i\|_\infty)^{2\nu_1}} - 1 \right] \right\}.$$

Further on, if $0 \leq \tilde{\omega}_i \leq 2/\|f_i\|_\infty$ then for all $v_{n_i} \in \mathbb{C}^{N_i}$ and $\nu_2 \in \mathbb{N}$

$$\|\tilde{S}_i^{\nu_2} v_{n_i}\|_A^2 \leq \|v_{n_i}\|_A^2 - \beta \|v_{n_i}\|_{A^2}^2$$

holds with

$$\beta \leq \frac{1 - (1 - \tilde{\omega}_i \|f_i\|_\infty)^{2\nu_2}}{\|f_i\|_\infty}.$$

Proof. See [6]. □

Regarding the choice of the coarse level we assume that the number of unknowns in each "direction" is divisible by 2, i.e. $(n_i)_j \bmod 2 = 0$ for $j = 1, \ldots, d$. We then on the coarse level choose every other degree of freedom, effectively dividing the number of unknowns by 2^d when moving from level i to level $i+1$. This corresponds to standard coarsening in geometric multigrid. Other coarsenings, e.g. by a factor different from 2 [13] or corresponding to semi-coarsening [14, 15] are derived and used in a straightforward way. The reduction from the fine level to the coarse level is described with the help of a *cut matrix* $K_{n_i} \in \mathbb{C}^{n_{i+1} \times n_i}$ that in the case of even system size on the fine level and of a 1-level circulant matrix is given by

$$K_{n_i} = \begin{bmatrix} 1 & 0 & & & & & \\ & & 1 & 0 & & & \\ & & & & \ddots & & \\ & & & & & 1 & 0 \end{bmatrix}.$$

The effect of this cut matrix is that every even variable is skipped when it is transferred to the coarse level. Regarding the action of the cut matrix on the Fourier matrix we obtain

$$K_{n_i} F_{n_i} = \frac{1}{\sqrt{2}}[1,1] \otimes F_{n_{i+1}} = \frac{1}{\sqrt{2}} F_{n_{i+1}}([1,1] \otimes I_{n_{i+1}}) \tag{8}$$

in the 1-level case. In the d-level case the cut matrix is defined by Kronecker product

$$K_{n_i} = K_{(n_i)_1} \otimes \cdots \otimes K_{(n_i)_d}. \tag{9}$$

Combining (8) with (9) and due to the properties of the Kronecker product we have

$$\begin{aligned} K_{n_i} F_{n_i} &= K_{(n_i)_1} F_{(n_i)_1} \otimes \cdots \otimes K_{(n_i)_d} F_{(n_i)_d} \\ &= \frac{1}{\sqrt{2^d}} (F_{(n_{i+1})_1}([1,1] \otimes I_{(n_{i+1})_1})) \otimes \cdots \otimes (F_{(n_{i+1})_d}([1,1] \otimes I_{(n_{i+1})_d})) \\ &= \frac{1}{\sqrt{2^d}} F_{n_{i+1}} \Theta_{n_{i+1}}, \end{aligned} \tag{10}$$

where $\Theta_{n_{i+1}} = ([1,1] \otimes I_{(n_{i+1})_1}) \otimes \cdots \otimes ([1,1] \otimes I_{(n_{i+1})_d})$. With the help of the cut matrix the prolongation is now defined as

$$P_i = \mathcal{C}_{n_i}(p_i) K_{n_i}^T$$

given some generating symbol p_i and the restriction is defined as the adjoint of the prolongation. To show the approximation property, we first define the set $\Omega(x)$ of all "corners" of x, given by

$$\Omega(x) = \{y : y_j \in \{x_j, x_j + \pi\}\},$$

and the set $\mathcal{M}(x)$ of all "mirror points" of x as

$$\mathcal{M}(x) = \Omega(x) \backslash \{x\}.$$

To obtain optimal, i.e. level independent, multigrid convergence the generating symbol p_i of the prolongation has to fulfill certain properties. For that purpose let x^0 in $[-\pi, \pi)^d$ be the single isolated zero of the generating symbol f_i of the system matrix on level i. Choose p_i such that

$$\limsup_{x \to x^0} \left| \frac{p_i(y)}{f_i(x)} \right| < +\infty, \qquad y \in \mathcal{M}(x), \quad i = 0, \ldots, l_{\max} - 1 \tag{11}$$

and such that for all $x \in [-\pi, \pi)$ we have

$$0 < \sum_{y \in \Omega(x)} |p_i|^2(y), \qquad i = 0, \ldots, l_{\max} - 1. \tag{12}$$

Using this, the approximation property can be stated for circulant matrices.

Theorem 2.2. *Let $A_i = \mathcal{C}_{n_i}(f_i)$ with f_i being the d-variate nonnegative generating symbol of A_i, having a single isolated zero in $[-\pi, \pi)^d$, let M_i be as in* (4)*, with $P_i = \mathcal{C}_{n_i}(p_i)K_{n_i}^H$ and $R_i = P_i^H$. If p_i fulfills* (11) *and* (12)*, then there exists a $\mu > 0$ such that for all $v_{n_i} \in \mathbb{C}^{N_i}$ we have*

$$\|M_i v_{n_i}\|_{A_i}^2 \leq \mu \|v_{n_i}\|_{A_i^2}^2.$$

Proof. See [6]. □

If the order of the zero x^0 of the generating symbol is $2q$, p_i is usually being chosen as

$$p_i(x) = c \cdot \prod_{j=1}^{d} (\cos(x_j^0) + \cos(x_j))^q,$$

plus optionally a Strang correction.

If the system matrix A is not circulant but Toeplitz, a few changes are necessary. In the case of a Toeplitz matrix which has a generating symbol f being a trigonometric polynomial of degree at most one, the matrix is in the τ-algebra. Matrices out of the τ-algebra are diagonalized by the matrix Q_n,

$$(Q_n)_{j,k} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{jk\pi}{n+1}\right), \qquad j, k = 1, \ldots, n.$$

Assuming n_i odd, the cut matrix K_{n_i} is chosen as

$$K_{n_i} = \begin{bmatrix} 0 & 1 & 0 & & & & \\ & & & 1 & 0 & & \\ & & & & & \ddots & \\ & & & & & 1 & 0 \end{bmatrix} \tag{13}$$

in the τ-case, the results on multilevel matrices and convergence transfer to this case immediately, if Q_n is chosen instead of F_n and the appropriate cut matrix is used. If A is Toeplitz but the generating symbol is a higher degree trigonometric polynomial of degree δ, the cut matrix has to be chosen as

$$K_{n_i}(\delta) = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & & & & & \\ & & & & & 1 & 0 & & & \\ & & & & & & & \ddots & & \\ & & & & & & & 1 & 0 & \cdots & 0 \end{bmatrix}, \tag{14}$$

where the first and last δ columns are zero, so the non-constant entries in the first δ and in the last δ rows and columns are not taken into account on the coarser level to guarantee the Toeplitz structure on all levels.

We will now focus on the choice of p_i in an aggregation based framework.

3. Aggregation and smoothed aggregation for circulant and Toeplitz matrices

Aggregation based multigrid goes back at least to [16], where the so-called aggregation/disaggregation methods [17, 18] have been used in a multigrid setting. The idea of aggregation based multigrid is to not choose a C/F-splitting, i.e. a partitioning of the unknowns into variables that are present on the coarse and the fine level and variables that are present on the fine level, only. Rather than that the unknowns are grouped together into *aggregates*, these aggregates form one variable on the coarse level, each. The pure aggregation can be improved by smoothing [19] that improves the quality of the prolongation and restriction and thus the performance of the method. Recent results on aggregation-based multigrid methods can be found in [20, 21]. In the following, we will start with the definition of simple aggregation based multigrid methods for 1-level circulant matrices, corresponding to one dimensional problems. Emphasizing the downside of pure aggregation we will then introduce smoothed aggregation in the circulant setting and finally transfer the results to the d-level case.

3.1. 1-level circulant matrices

Let $A = \mathcal{C}_n(f)$ with generating symbol f having a single isolated zero of order 2 at the origin, $n = 2^{l_{\max}+1}$. In an aggregation-based multigrid method with aggregates of size 2 this corresponds to a prolongation operator P_i given by

$$P_i^H = \begin{bmatrix} 1 & 1 & & & & & \\ & & 1 & 1 & & & \\ & & & & \ddots & & \\ & & & & & 1 & 1 \end{bmatrix} \in \mathbb{C}^{n_{i+1} \times n_i}.$$

Transferring this to the circulant case yields a prolongation $P_i = \mathcal{C}_{n_i}(p_i) K_{n_i}^T$ with $p_i = a_{1,2}$, where

$$\begin{aligned} a_{1,2} : [-\pi, \pi) &\to \mathbb{C} \\ x &\mapsto a_{1,2}(x) = 1 + \mathrm{e}^{-\mathrm{i}x}. \end{aligned}$$

Note that $\mathcal{C}_{n_i}(p_i)$ is not hermitian. We easily check that this projector fulfills (12) as

$$\begin{aligned}\sum_{y\in\Omega(x)} |p_i(y)|^2 &= \sum_{y\in\Omega(x)} |1+\mathrm{e}^{-\mathrm{i}y}|^2 \\ &= \sum_{y\in\Omega(x)} 2+2\cos(y) > 0\end{aligned}$$

This projection does not fulfill (11), but as f has a second-order zero at $x^0 = 0$, we can show that it fulfills a weaker condition sufficient for two-grid optimality, namely

$$\limsup_{x\to x^0} \frac{|p_i(y)|^2}{|f_i(x)|} \le +\infty, \qquad y \in \mathcal{M}(x), \qquad i = 0,\dots,l_{\max}-1. \tag{15}$$

Therefore the aggregation defines an optimal two-grid method but it is not strong enough for the optimality of V-cycle. This agrees with results in [20].

To fulfill the stronger condition (11) the prolongation can be improved by smoothing, i.e. applying a step of an iterative method used as a smoother. In the case of Richardson this corresponds to the generating symbol

$$s_{i,\omega}(x) = 1 - \omega f_i(x). \tag{16}$$

Under the assumption that f_i has its single maximum at position $x = \pi$ no additional zero is introduced when ω is chosen as $\omega = 1/f(\pi)$ and the symbol of the prolongation operator

$$p_i(x) = s_{i,1/f(\pi)}(x)\, a_{1,2}(x)$$

fulfills (11) since $s_{i,1/f(\pi)}(\pi) = 0$.

We like to note that if the introduced zero is of second order it suffices to smooth either the prolongation or the restriction operator, as the symbol of the pure aggregation already has a zero of order 1 at the mirror point $x = \pi$. Since in this case $R_i \neq P_i$ the previous theory does not apply. Nevertheless, defining $R_i = K_{n_i}\mathcal{C}_{n_i}(r_i)$, in [22] it is shown that the condition (12) can be replaced with

$$0 < \sum_{y\in\Omega(x)} r_i(y)p_i(y), \qquad i = 0,\dots,l_{\max}-1. \tag{17}$$

and the two-grid condition (15) replaced with

$$\limsup_{x\to x^0} \frac{|r_i(y)p_i(y)|}{|f_i(x)|} \le +\infty, \qquad y \in \mathcal{M}(x), \qquad i = 0,\dots,l_{\max}-1. \tag{18}$$

Similarly, assuming that $r_ip_i \ge 0$, the condition (11) can be replaced with

$$\limsup_{x\to x^0} \left|\frac{\sqrt{r_i(y)p_i(y)}}{f_i(x)}\right| < +\infty, \qquad y \in \mathcal{M}(x), \quad i = 0,\dots,l_{\max}-1. \tag{19}$$

The coarse matrix $A_{i+1} = R_i A_i P_i$ is $A_{i+1} = \mathcal{C}_n(f_{i+1})$ with

$$f_{i+1}(x) = \frac{1}{2} \sum_{y \in \Omega(x/2)} r_i(y) f_i(y) p_i(y)$$

and hence it is nonnegative definite for $r_i p_i \geq 0$. Smoothing only the restriction or the prolongation operator, we have

$$r_i(x)p_i(x) = s_{i,\omega}(x)a_{1,2}(x)\overline{a_{1,2}(x)} = s_{i,\omega}(x)(2 + 2\cos(x)).$$

Under the assumption that f has maximum at π, $s_{i,1/f(\pi)}$ is nonnegative and has a zero of order 4 at π. Hence conditions (17) and (19) are satisfied and A_{i+1} is nonnegative definite.

Remark 3.1. *This choice of p_i is only valid for system matrices $A = \mathcal{C}_n(f)$ where the generating symbol has a single isolated zero at $x_0 = 0$. In general for a system matrix with generating symbol f_i having a single isolated zero at x_0 we choose p_i as*

$$\begin{aligned} p_i : [-\pi, \pi) &\to \mathbb{C} \\ x &\mapsto p_i(x) = 1 + \mathrm{e}^{-\mathrm{i}(x+x_0)}. \end{aligned}$$

For this prolongation operator we have

$$|p_i(x)|^2 = 2 + 2\cos(x + x_0),$$

so (12) *and* (15) *are fulfilled, the latter for a single isolated zero x_0 of order 2. The stronger condition* (11) *is fulfilled in the case that f_i has its single maximum at $x_0 + \pi$ by smoothing the operator using ω-Richardson with $\omega = f_i(x_0 + \pi)$.*

In general, aggregation with aggregates of sizes g corresponds to using the cut matrix

$$K_{n_i,g} = \begin{bmatrix} 1 & 0 & \cdots & 0 & & & & & & & & \\ & & & & 1 & 0 & \cdots & 0 & & & & \\ & & & & & & & & \ddots & & & \\ & & & & & & & & & 1 & 0 & \cdots & 0 \end{bmatrix} \tag{20}$$

with $g - 1$ zero columns after each column containing a one and the prolongation defined by this cut matrix and the generating symbol $p_i = a_{1,g}$ with

$$\begin{aligned} a_{1,g} : [-\pi, \pi) &\to \mathbb{C} \\ x &\mapsto a_{1,g}(x) = \sum_{k=0}^{g-1} \mathrm{e}^{-\mathrm{i}kx} \end{aligned}$$

as

$$P_i = \mathcal{C}_{n_i}(p_i) K_{n_i,g}^T. \tag{21}$$

The effect of the cut matrix applied to the Fourier matrix is similar to (8) described by

$$K_{n_i,g} F_{n_i} = \frac{1}{\sqrt{g}} e_g^T \otimes F_{n_{i+1}} = \frac{1}{\sqrt{g}} F_{n_{i+1}} (e_g^T \otimes I_{n_{i+1}}),$$

where $e_g^T = [1, \ldots, 1] \in \mathbb{N}^g$ and the set of mirror points consists of the $g-1$ points in $\mathcal{M}_g(x) = \Omega_g(x) \backslash \{x\}$ where

$$\Omega_g(x) = \left\{ y : y = x + \frac{2\pi j}{g} (\mathrm{mod} 2\pi),\ j = 0, 1, \ldots, g-1 \right\}.$$

Assuming $n_0 = n = g^{l_{\max}+1}$, for a given matrix $A_i = \mathcal{C}_{n_i}(f_i)$ the coarse level matrix $A_{i+1} = P_i^H A_i P_i$, $n_{i+1} = n_i/g$ is given by $A_{i+1} = \mathcal{C}_{n_{i+1}}(f_{i+1})$ with

$$f_{n_{i+1}}(x) = \frac{1}{g} \sum_{y \in \Omega_g(x/g)} |p|^2 f(y), \qquad x \in [-\pi, \pi).$$

For further details see [13], where it is proved that the two-grid convergence follows as in the case $g = 2$ outlined in section 2 with the requirements (15) and (12) stated on the sets $\mathcal{M}_g$ and Ω_g, respectively. In more detail, the two-grid optimality requires

$$\limsup_{x \to x^0} \frac{|p_i(y)|^2}{|f_i(x)|} \leq +\infty, \qquad y \in \mathcal{M}_g(x), \quad i = 0, \ldots, l_{\max} - 1, \tag{22}$$

$$0 < \sum_{y \in \Omega_g(x)} |p_i|^2(y), \qquad i = 0, \ldots, l_{\max} - 1, \tag{23}$$

for all $x \in [-\pi, \pi)$, see Theorem 5.1 in [13]. The V-cycle optimality for a coarsening factor $g > 2$ is an open problem, but we can conjecture that in (11), similarly to (15), it is enough to replace $\mathcal{M}$ with $\mathcal{M}_g$, namely

$$\limsup_{x \to x^0} \left| \frac{p_i(y)}{f_i(x)} \right| < +\infty, \qquad y \in \mathcal{M}_g(x), \quad i = 0, \ldots, l_{\max} - 1. \tag{24}$$

As the pure aggregation $p_i = a_{1,g}$ fulfills only (22) but not (24), the prolongation has to be improved for all mirror points, possibly resulting in more than one smoothing parameter ω and thus multiple necessary smoothing steps. The extension to the case of zeros at other positions is possible analogously to the case outlined in Remark 3.1 with the same symbol $p_i(x) = 1 + \mathrm{e}^{-\mathrm{i}(x+x_0)}$.

3.2. The d-level case

Using the 1-level case as motivation, we will now introduce aggregation and smoothed aggregation multigrid for d-level circulant matrices, $d \in \mathbb{N}$, usually associated to d-dimensional problems. First of all, we have to extend the theoretical results in [13] to $d > 1$. For that purpose let $A = \mathcal{C}_n(f)$, where $f : \mathbb{R}^d \to \mathbb{C}$ is a nonnegative function 2π-periodic in each variable, $n \in \mathbb{N}^d$, $g \in \mathbb{N}^d$ is the size of the aggregates and assume that $n = g^{l_{\max}+1}$, i.e., $n_j = g_j^{l_{\max}+1}$, $j = 1, \ldots, d$. As before, we define the fine level operator $A_0 = A$ with $f_0 = f$ and recursively the system size as $n_{i+1} = n_i/g$ (all the multi-indices operations in the paper are intended component-wise), the prolongation as in (21) where $K_{n_i,g} = K_{(n_i)_1,g_1} \otimes \cdots \otimes K_{(n_i)_d,g_d}$, and the coarse grid operator as $A_{i+1} = P_i^H A_i P_i$. The set of all corners of $x \in \mathbb{R}^d$ associated to the cut matrix $K_{n_i,g}$ is

$$\Omega_g(x) = \left\{ y \;\middle|\; y_j \in \left\{ x_j + \frac{2\pi k}{g_j} \pmod{2\pi} \right\}, \, k = 0, \ldots, g_j - 1, \, j = 1, \ldots, d \right\}.$$

To simplify the following notation we define $G = \prod_{j=1}^{d} g_j$.

Analogously to the 1-level case, the generating symbol of the system matrix of the coarser level is given as stated by the following lemma.

Lemma 3.2. *Let $A_i = \mathcal{C}_{n_i}(f_i)$, P_i defined in (21), and $n_{i+1} = g \cdot n_i \in \mathbb{N}^d$, then the coarse level system matrix $A_{i+1} = P_i^H A_i P_i$ is $A_{i+1} = \mathcal{C}_{n_{i+1}}(f_{i+1})$ where*

$$f_{i+1}(x) = \frac{1}{G} \sum_{y \in \Omega_g(x/g)} |p_i|^2 f_i(y), \qquad x \in [-\pi, \pi)^d. \tag{25}$$

Proof. The proof is a generalization of the proof of Proposition 5.1 in [4]. First we note that in analogy to (10) with $e_{g_j}^T = [1, \ldots, 1] \in \mathbb{N}^{g_j}$, $j = 1, \ldots, d$, we have

$$\begin{aligned} K_{n_i,g} F_{n_i} &= K_{(n_i)_1,g_1} F_{n_{i,1}} \otimes \cdots \otimes K_{(n_i)_d,g_d} F_{n_{i,d}} \\ &= \frac{1}{\sqrt{G}} (F_{n_{i+1,1}} (e_{g_1}^T \otimes I_{n_{i,1}})) \otimes \cdots \otimes (F_{n_{i+1,d}} (e_{g_d}^T \otimes I_{n_{i,d}})) \\ &= \frac{1}{\sqrt{G}} (F_{n_{i+1,1}} \otimes \cdots \otimes F_{n_{i+1,d}}) ((e_{g_1}^T \otimes I_{n_{i,1}}) \otimes \cdots \otimes (e_{g_d}^T \otimes I_{n_{i,d}})), \end{aligned}$$

so

$$K_{n_i} F_{n_i} = \frac{1}{\sqrt{G}} F_{n_{i+1}} \Theta_{n_i,g}, \tag{26}$$

where $\Theta_{n_i,g} = (e_{g_1}^T \otimes I_{n_{i,1}}) \otimes \cdots \otimes (e_{g_d}^T \otimes I_{n_{i,d}})$. So, for $A_{i+1} = P_i^H A_i P_i$ we have

$$\begin{aligned} P_i^H A_i P_i &= K_{n_i,g} \mathcal{C}_{n_i}^H(p_i) \mathcal{C}_{n_i}(f_i) \mathcal{C}_{n_i}(p_i) K_{n_i,g}^H \\ &= K_{n_i,g} F_{n_i} D_{n_i}(|p_i|^2 f_i) F_{n_i}^H K_{n_i,g}^H \\ &= \frac{1}{G} F_{n_{i+1}} \Theta_{n_i,g} D_{n_i}(|p_i|^2 f_i) \Theta_{n_i,g}^H F_{n_{i+1}}^H. \end{aligned}$$

Here,

$$D_{n_i}(f) = \text{diag}_{0\le j\le n_i-e_d}(f((x_i)_j)),$$

where $(x_i)_j \equiv 2\pi j/n_i = (2\pi j_1/(n_i)_1, \ldots, 2\pi j_d/(n_i)_d)^T$ and $0 \le j \le n_i - e_d$ is intended component-wise. For a given multi-index $k = (k_1, \ldots, k_d)$, $0 \le k_j \le (n_{i+1})_j$ we have

$$(\Theta_{n_i,g}x)_k = \sum_{l=0}^{g-e_d} x_{k+l},$$

so we obtain

$$\Theta_{n_i,g}D_{n_i}(|p_i|^2 f_i)\Theta_{n_i,g}^T = \sum_{l=0}^{g-e_d} D_{n_i,g,l}(|p_i|^2 f_i),$$

where

$$D_{n_i,g,l}(f) = \text{diag}_{n_{i+1}\cdot l\le j'\le n_{i+1}\cdot(l+e_d)-e_d}(f((x_i)_{j'})).$$

Here the products and inequalities are again intended component-wise. For an example of the multi-index notation in the case $d = g = 2$ we refer to the proof of Proposition 5.1 in [4]. As result we obtain

$$P_i^H A_i P_i = \frac{1}{G} F_{n_{i+1}} \left(\sum_{l=0}^{g-e_d} D_{n_i,g,l}(|p_i|^2 f_i) \right) F_{n_{i+1}}^H$$

and with

$$(x_i)_{j'} = (x_{i+1})_j/g + \pi \cdot l \pmod{2\pi}, 0 \le j \le n_{i+1} - e_d, j' = j + n_{i+1}\cdot l,$$

where products, divisions and inequalities are intended component-wise, we get

$$P_i^H A_i P_i = \mathcal{C}_{n_{i+1}}(f_{i+1}),$$

with f_{i+1} defined in (25).

□

The two-grid optimality can be obtained similarly to the 1-level case if the conditions (22) and (23) are satisfied for $x \in [-\pi, \pi)^d$. The proof is a combination of Theorem 5.1 in [13] and Lemma 6.3 in [4]. It requires a quite complicate notation, but the main point is the standard reduction, by proper permutations, to a diagonal blocks matrix with diagonal blocks of size $G \times G$. The boundedness of the modulus of the entries, and hence the boundedness of the norm of the matrix, follows from conditions (22) and (23).

Remark 3.3. *If the two conditions* (22) *and* (23) *are satisfied with* $x \in [-\pi, \pi)^d$*, we obtain as consequence of Lemma 3.2 that if* x^0 *is a zero of* f_i *then* $g \cdot x^0 \bmod 2\pi$ *is a zero of* f_{i+1} *with the same order.*

In the pure aggregation setting the generating symbol of the prolongation is given by

$$a_{d,g}(x) = \prod_{j=1}^{d} \sum_{k=0}^{g_j-1} \mathrm{e}^{-\mathrm{i}kx_j}, \qquad x \in [-\pi, \pi)^d. \tag{27}$$

Theorem 3.4. *For the function $a_{d,g}$ defined in* (27) *there exists a constant c with $0 < c < +\infty$ such that*

$$\limsup_{x\to 0} \frac{|a_{d,g}(y)|}{\sum_{j=1}^{d} x_j^z} = c, \qquad y \in \mathcal{M}_g(x). \tag{28}$$

where $z = d - \#\{y_j \,|\, y_j = 0,\ j = 1, \ldots, d\}$ is the number of directions along which $a_{d,g}$ is zero.
Further on, if f_i has a single isolated zero of order 2 at the origin, $p_i = a_{d,g}$ fulfills (23) *and* (22)*.*

Proof. The limit (28) follows from the Taylor series of $a_{d,g}$: Consider $y \in \mathcal{M}_g(x)$, i.e., $y_j = x_j + \frac{2\pi\ell}{g_j} \pmod{2\pi}$ for $\ell = 0, \ldots, g_j - 1$, then the j-th factor of $a_{d,g}(y)$ is

$$\sum_{k=0}^{g_j-1} \mathrm{e}^{-\mathrm{i}ky_j} = \sum_{k=0}^{g_j-1} \mathrm{e}^{-\mathrm{i}k(x_j + \frac{2\pi\ell}{g_j})} = \sum_{k=0}^{g_j-1} \mathrm{e}^{\frac{-\mathrm{i}2\pi k\ell}{g_j}} \mathrm{e}^{-\mathrm{i}kx_j}.$$

Since

$$\sum_{k=0}^{g_j-1} \mathrm{e}^{\frac{-\mathrm{i}2\pi k\ell}{g_j}} = \begin{cases} g_j & \text{if } \ell = 0, \\ 0 & \text{otherwise,} \end{cases}$$

the j-th factor in (27) has an infinite Taylor series with the constant term equal to zero only if $\ell \neq 0$.
If f_i has a single isolated zero of order 2 at the origin then

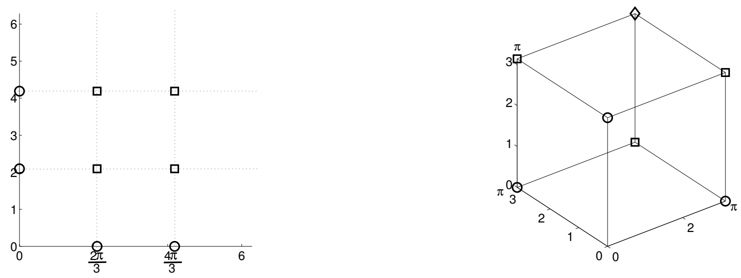
$$\limsup_{x\to 0} \frac{f_i(x)}{\sum_{j=1}^{d} x_j^2} = \hat{c}, \qquad 0 < \hat{c} < +\infty$$

and hence $p_i = a_{d,g}$ fulfills (22).

Regarding (23), let x be such that $|a_{d,g}|^2(x) = 0$. If x lies on the axes then $0 \in \Omega_g(x)$ and $|a_{d,g}|^2(0) > 0$. If x does not lie on the axes, then there exists a $y \in \Omega_g(x)$ that lies on an axis and that fulfills $|a_{d,g}|^2(y) > 0$. □

Figure 1 gives a visual representation of the behaviour of $p_i = a_{d,g}$ at $\mathcal{M}_g(0)$ for two examples.

The order of the zero at the points where $p_i = a_{d,g}$ is zero in one direction, only, can again be improved by applying smoothing. For that purpose we



$d = 2,\ g = (3, 3)$ $\qquad$ $d = 3,\ g = (2, 2, 2)$

Figure 1: Order of $y \in \mathcal{M}_g(0)$ for the aggregation operator $a_{d,g}$: $\circ \to$ order $= 1$, $\square \to$ order $= 2$, $\Diamond \to$ order $= 3$.

again use an ω-Richardson smoother. In the d-level case the generating symbol of this smoother is given by

$$s_{i,\omega} : [-\pi, \pi)^d \to \mathbb{C} \tag{29}$$

$$x \to s_{i,\omega}(x) = 1 - \omega f_i(x). \tag{30}$$

Lemma 3.5. *Assume that $f_i \geq 0$ has a single isolated zero of order 2 at the origin and that f_i obtains the maximum only at all $y \in \mathcal{M}_g(0)$ lying on the axes and let $\tilde{y}$ be one of these points. Then the symbol of the smoothed prolongation given by*

$$p_i(x) = s_{i,1/f(\tilde{y})}(x)\, a_{d,g}(x)$$

fulfills (24) *and* (23)*.*

Proof. Since $\tilde{y}$ is of maximum for f_i, the function $s_{i,1/f(\tilde{y})}$ is nonnegative and vanishes for $y \in \mathcal{M}_g(0)$ lying on the axes with order at least one. From Theorem 3.4 $a_{d,g}$ vanishes at $y \in \mathcal{M}_g(0)$ with order one if y lies on the axes and with order at least two, otherwise. Therefore, $p_i = s_{i,1/f(\tilde{y})}\, a_{d,g}$ vanishes with order at least two for all $y \in \mathcal{M}_g(0)$ and hence it fulfills (24).

Regarding (23), the assumptions on f_i implies that $s_{i,1/f(\tilde{y})}(y) = 0$ only for $y \in \mathcal{M}_g(0)$ lying on the axes. Hence $\{x \mid s_{i,1/f(\tilde{y})}(x) = 0\} \subset \{x \mid a_{d,g}(x) = 0\}$ and $p_i = a_{d,g} s_{i,1/f(\tilde{y})}$ fulfills (23) since it is already satisfied by $p_i = a_{d,g}$ thanks to Theorem 3.4. $\square$

Again, if the smoother introduces a zero of order two, it is sufficient to smooth either the prolongation or the restriction operator generalizing the results in [22] to $g > 2$. Moreover, like in Remark 3.1 the aggregation operator for a zero at a position $x^0 \neq 0 \in \mathbb{R}^d$ is defined by

$$p_i(x) = \prod_{j=1}^{d} \sum_{k=0}^{g_j - 1} \mathrm{e}^{-\mathrm{i}k(x_j + x_j^0)}, \qquad x \in [-\pi, \pi)^d.$$

Now we turn to discretizations of the two-dimensional Laplacian. In this case we are able to formulate some results based on the developed theory. The first result is valid for isotropic stencils in the case of standard coarsening.

Lemma 3.6. *Let f be an even trigonometric polynomial obtained by an isotropic discretization of the 2D Laplacian. If $g = (2, 2)$ or $g = (3, 3)$, (i.e., coarsening $1 : 2$ and $1 : 3$, respectively, in x- and y-direction), there always exists a smoother $s_{i,\omega}$ defined in (29) with unique ω such that the resulting projection $p_i = s_{i,\omega}\, a_{2,g}$ fulfills (24). In particular*

i) for $g = (2, 2)$ we obtain $\omega = 1/f(0, \pi)$,

ii) for $g = (3, 3)$ we obtain $\omega = 1/f(0, \frac{2\pi}{3})$.

Proof. The function f is nonnegative and vanishes only at the origin with order two, thus p_0 has to vanish at all $y \in \mathcal{M}_g(0)$ with order at least two. For $y \in \mathcal{M}_g(0)$, from Theorem 3.4 the aggregation part $a_{2,g}$ vanishes in y with order one if y lies on the axes and with order two otherwise. The isotropic discretization leads to a symmetry on f such that $f(0, z) = f(z, 0)$, that is inherited by $s_{0,\omega}$. For $g = (2, 2)$, the smoother $s_{i,\omega}$ can be defined with one unique ω leading to $s_{0,\omega}(0, \pi) = 1 - \omega f(0, \pi) = 0$. For $g = (3, 3)$, we observe that $\cos(4\pi/3) = \cos(2\pi/3)$ and hence the smoother $s_{i,\omega}$ can be again defined with one unique ω leading to $s_{0,\omega}(0, 4\pi/3) = s_{0,\omega}(0, 2\pi/3) = 1 - \omega f(0, 2\pi/3) = 0$. The coarse symbols f_i, $i > 0$, preserve the same properties of f thanks to Lemma 3.2 and Remark 3.3. □

In the case that every fourth point is taken in each direction, i.e. the number of unknowns is reduced by a factor of 16, we obtain a similar result.

Lemma 3.7. *Let f be an even trigonometric polynomial obtained by an isotropic discretization of the 2D Laplacian. If $g = (4, 4)$ (i.e., coarsening $1 : 4$ in x- and y-direction), we need two smoothers with two different ω given by $\omega_1 = 1/f(0, \pi/2)$ and $\omega_2 = 1/f(0, \pi)$ such that the resulting projection $p_i = s_{i,\omega_1} s_{i,\omega_2}\, a_{2,g}$ fulfills (24).*

Proof. The proof is analogous to that of Lemma 3.6. Two different ω are necessary in view of $\cos(\pi/2) = \cos(3\pi/2) \neq \cos(\pi)$. The smoother s_{i,ω_1} can be defined by $s_{0,\omega_1}(0, \pi/2) = 1 - \omega_1 f(0, \pi/2) = 0$, while the smoother s_{i,ω_2} can be defined by $s_{0,\omega_2}(0, \pi) = 1 - \omega_2 f(0, \pi) = 0$ □

For anisotropic stencils even with standard coarsening in general two ω are needed.

Lemma 3.8. *Let f be an anisotropic discretization of the 2D Laplacian. If $g = (2, 2)$ (i.e., coarsening $1 : 2$ in x- and y-direction), we need two different ω given by $\omega_1 = 1/f(\pi, 0)$ and $\omega_2 = 1/f(0, \pi)$ such that the resulting projection $p_i = s_{i,\omega_1} s_{i,\omega_2}\, a_{2,g}$ fulfills (24).*

Proof. Due to the anisotropic discretization $f(\pi, 0) \neq f(0, \pi)$ and hence two different ω are necessary like in Lemma 3.7. $\square$

3.3. Toeplitz case

As noted at the end of section 2 the circulant case can be applied and extended to the Toeplitz case. In analogy to (13) the cut matrix $K_{n_i,g}$ given by (20) in the Toeplitz case is given by

$$K_{n_i,g} = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & & & & & & & & \\ & & & & & & & 1 & 0 & \cdots & 0 & & & & \\ & & & & & & & & & & & \ddots & & & \\ & & & & & & & & & & & & 1 & 0 & \cdots & 0 \end{bmatrix},$$

where the first and last $g-1$ columns are zero. The multilevel counterpart is formed with the help of Kronecker products. In the case that the degree of the trigonometric polynomial is smaller than g in the 1-level case of the degree of each variable in the multilevel case is smaller than the corresponding g_j the Toeplitz structure is kept on the coarser levels. This is a general advantage of multigrid methods that use reductions of the system size that are different from 2. If the degree is higher the cut matrix can be padded with zeros as in (14).

3.4. Non-constant coefficient case

While non-constant coefficients do not lead to circulant or Toeplitz matrices, circulant or Toeplitz matrices can be used as a local model by freezing the coefficients and analyzing the resulting methods. This approach is followed in [22] and in general when local Fourier analysis (LFA) for multigrid methods is used to analyze geometric multigrid methods. For a detailed review of LFA see [23]. The developed theory can be used to choose different smoothers based on the local stencil within the smoothing process in general smoothed aggregation multigrid methods. This is beyond the scope of this paper and will be considered in future investigations.

4. Numerical examples

All numerical tests were obtained using MATLAB R2011b. We implemented the outlined method based on the developed theory for circulant and Toeplitz d-level matrices with generating symbols with second order zero at the origin. The optimal ω was chosen automatically according to lemmas 3.6–3.8. In any case we used 3 steps each of the Richardson iteration as pre- and postsmoother. Unless indicated otherwise the coarsest grid was of size 2^d. We report the number iterations to yield a reductions of the residual by a factor of 10^{-10}, the operator complexity and the asymptotic convergence rate given by the residuals of the last two cycles.

# dof	# iter.	op. compl.	asymp. conv.
2^2	6	1.3333	0.0156
2^3	6	1.8333	0.0156
2^4	6	2.2500	0.0189
2^5	6	2.6250	0.0181
2^6	10	2.8542	0.1828
2^7	9	3.0938	0.1793
2^8	9	3.3177	0.1813

Table 1: Results for the circulant case for stencil (31) for a coarsening by 1:2.

# dof	# iter.	op. compl.	asymp. conv.
2^2	6	1.3333	0.0156
2^3	7	1.6667	0.0568
2^4	8	1.8333	0.0763
2^5	8	1.9167	0.0703
2^6	8	1.9583	0.0686
2^7	8	1.9792	0.0686
2^8	8	1.9896	0.0786

Table 2: Results for the circulant case for stencil (31) for a coarsening by 1:2 (non-Galerkin case).

4.1. 1-level example

As a simple 1-level example we consider the 2nd-order accurate discretization of the Laplace operator given by the stencil

$$\begin{bmatrix} -1 & 2 & -1 \end{bmatrix} \tag{31}$$

that corresponds to the generating symbol

$$f(x) = 2 - 2\cos(x).$$

If the operator is discretized with periodic boundary conditions we obtain the circulant matrix given by this generating symbol, when Dirichlet boundary conditions are used, the respective Toeplitz matrix is obtained. We observe that f attains its single maximum at $x_{\max} = \pi$, so the requirement of Lemma 3.5 is fulfilled. The results for a reduction ratio of two for the circulant case can be found in Table 1. Only one ω was needed on each grid level. The operator complexity is growing strongly, a behavior that can be reduced by smoothing one grid transfer operator, only, as discussed above. The results obtained in the non-Galerkin case where only the prolongation operator is smoothed can be found in Table 2. The other option to reduce

# dof	# iter.	op. compl.	asymp. conv.
3^2	12	1.3333	0.1584
3^3	13	1.4444	0.1766
3^4	12	1.4815	0.1822
3^5	12	1.4938	0.1783

Table 3: Results for the circulant case for stencil (31) for a coarsening by 1:3.

# dof	# iter.	op. compl.	asymp. conv.
$3^2 - 1$	12	1.1818	0.1763
$3^3 - 1$	13	1.3421	0.1976
$3^4 - 1$	12	1.4286	0.1795
$3^5 - 1$	12	1.4696	0.1794

Table 4: Results for the Toeplitz case for stencil (31) for a coarsening by 1:3.

the operator complexity is a more aggressive coarsening that translates to larger aggregates. In Table 3 the results for stencil (31) can be found for a reduction ratio of 3. While the operator complexity is obviously lower than in the previous case, still only one ω is needed and the convergence rate is still satisfactory and independent of the size of the system. The results for the Toeplitz case are very similar to those in the circulant case, they are presented in Table 4.

Another example is the 4th-order discretization of the Laplacian corresponding to the stencil

$$\begin{bmatrix}1 & -16 & 30 & -16 & 1\end{bmatrix} \tag{32}$$

and having the generating symbol

$$f(x) = 30 - 32\cos(x) + 2\cos(2x).$$

The results obtained for a reduction ratio of 3 for circulant matrices with this stencil can be found in Table 5. Again, only one ω is needed.

# dof	# iter.	op. compl.	asymp. conv.
3^2	14	1.2000	0.2324
3^3	16	1.4000	0.2581
3^4	16	1.4667	0.2690
3^5	16	1.4889	0.2861

Table 5: Results for the circulant case for stencil (32) for a coarsening by 1:3.

# dof	# iter.	op. compl.	asymp. conv.
$3^2 \times 3^2$	20	1.2000	0.3581
$3^3 \times 3^3$	24	1.2222	0.4361
$3^4 \times 3^4$	23	1.2247	0.4354
$3^5 \times 3^5$	24	1.2250	0.4388

Table 6: Results for the circulant case for stencil (33) for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$(3^2-1)\times(3^2-1)$	24	1.0556	0.4043
$(3^3-1)\times(3^3-1)$	25	1.1526	0.4420
$(3^4-1)\times(3^4-1)$	25	1.1981	0.4431
$(3^5-1)\times(3^5-1)$	24	1.2156	0.4427

Table 7: Results for the Toeplitz case for stencil (33) for a coarsening by 1:9.

4.2. 2-level example

As a first example we choose the well-known 2nd-order accurate discretization of the Laplacian given by the stencil

$$\begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}. \tag{33}$$

The generating symbol is given by

$$f(x) = 4 - 2\cos(x_1) - 2\cos(x_2).$$

The results for a coarsening by a factor of 3 in each direction can be found in Table 6. The results for the Toeplitz case given in Table 7 are comparable. In any case, thanks to Lemma 3.6, only one ω is needed and the stencil is replicated on the coarse grid.

Another common example is the 2nd-order accurate 9-point discretization due to the finite element discretization of the Laplacian. It has the stencil

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}, \tag{34}$$

so the generating symbol is given by

$$f(x) = 8 - 2\cos(x_1) - 2\cos(x_2) - 4\cos(x_1)\cos(x_2),$$

it fulfills the requirements of Lemma 3.5. The results for the circulant case given in Table 8 and for the Toeplitz case given in Table 9 are similar to

# dof	# iter.	op. compl.	asymp. conv.
$3^2 \times 3^2$	14	1.1111	0.2286
$3^3 \times 3^3$	16	1.1235	0.2748
$3^4 \times 3^4$	16	1.1248	0.2786
$3^5 \times 3^5$	16	1.1250	0.2790

Table 8: Results for the circulant case for stencil (34) for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$(3^2-1) \times (3^2-1)$	16	1.0331	0.2571
$(3^3-1) \times (3^3-1)$	17	1.0866	0.2793
$(3^4-1) \times (3^4-1)$	17	1.1108	0.2840
$(3^5-1) \times (3^5-1)$	16	1.1200	0.2833

Table 9: Results for the Toeplitz case for stencil (34) for a coarsening by 1:9.

the case of the 5-point discretization and again just one ω is needed and the stencil stays the same on each level.

We now turn to an example where more than one ω is necessary. For that purpose we consider matrices with the stencil

$$\begin{bmatrix} -\frac{1}{12} & -\frac{6b-2a}{12a+12b} & -\frac{1}{12} \\ -\frac{6a-2b}{12a+12b} & 1 & -\frac{6a-2b}{12a+12b} \\ -\frac{1}{12} & -\frac{6b-2a}{12a+12b} & -\frac{1}{12} \end{bmatrix}, \tag{35}$$

yielding the symbol

$$f(x) = 1 - \frac{12a-4b}{12a+12b}\cos(x_1) - \frac{12b-4a}{12a+12b}\cos(x_2) - \frac{1}{3}\cos(x_1)\cos(x_2).$$

This corresponds to a discretization of an anisotropic PDE. According to Lemma 3.8, we need two ω to increase the order of the zero at the mirror points on the axes. First we consider an example with a slight anisotropy where we choose $a = 1$ and $b = 1.1$. The smoothing parameter ω was chosen automatically on each level and to reduce the growth of the operator complexity we choose to smooth the prolongation, only. The results for the circulant case can be found in Table 10 and for the Toeplitz case in Table 11. If the anisotropy is increased, the convergence rate deteriorates, as expected. The results for $a = 1$ and $b = 2$ can be found in Tables 12 for the circulant case and 13 for the Toeplitz case.

# dof	# iter.	op. compl.	asymp. conv.
$3^2 \times 3^2$	12	1.1111	0.2675
$3^3 \times 3^3$	18	1.1235	0.3436
$3^4 \times 3^4$	18	1.1248	0.3428
$3^5 \times 3^5$	18	1.1250	0.3451

Table 10: Results for the circulant case for the anisotropic stencil (35) with $a = 1$ and $b = 1.1$ for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$(3^2 - 1) \times (3^2 - 1)$	19	1.0331	0.3139
$(3^3 - 1) \times (3^3 - 1)$	19	1.0866	0.3480
$(3^4 - 1) \times (3^4 - 1)$	19	1.1108	0.3459
$(3^5 - 1) \times (3^5 - 1)$	19	1.1200	0.3467

Table 11: Results for the Toeplitz case for the anisotropic stencil (35) with $a = 1$ and $b = 1.1$ for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$3^2 \times 3^2$	22	1.1111	0.4137
$3^3 \times 3^3$	27	1.1235	0.4834
$3^4 \times 3^4$	26	1.1248	0.4819
$3^5 \times 3^5$	26	1.1250	0.4833

Table 12: Results for the circulant case for the anisotropic stencil (35) with $a = 1$ and $b = 2$ for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$(3^2 - 1) \times (3^2 - 1)$	25	1.0331	0.4251
$(3^3 - 1) \times (3^3 - 1)$	28	1.0866	0.4845
$(3^4 - 1) \times (3^4 - 1)$	27	1.1108	0.4869
$(3^5 - 1) \times (3^5 - 1)$	27	1.1200	0.4870

Table 13: Results for the Toeplitz case for the anisotropic stencil (35) with $a = 1$ and $b = 2$ for a coarsening by 1:9.

# dof	# iter.	op. compl.	asymp. conv.
$3^2 \times 3^2 \times 3^2$	14	1.0476	0.2286
$3^3 \times 3^3 \times 3^3$	15	1.0494	0.2694
$3^4 \times 3^4 \times 3^4$	15	1.0494	0.2727
$3^5 \times 3^5 \times 3^5$	15	1.0495	0.2734

Table 14: Results for the circulant case for stencil (36) for a coarsening by 1:27.

# dof	# iter.	op. compl.	asymp. conv.
$(3^2-1) \times (3^2-1) \times (3^2-1)$	15	1.0080	0.2305
$(3^3-1) \times (3^3-1) \times (3^3-1)$	17	1.0317	0.2787
$(3^4-1) \times (3^4-1) \times (3^4-1)$	17	1.0430	0.2832
$(3^5-1) \times (3^5-1) \times (3^5-1)$	16	1.0473	0.2854

Table 15: Results for the Toeplitz case for stencil (36) for a coarsening by 1:27.

4.3. 3-level example

To show the feasibility of the approach for 3-dimensional problems, we tested the approach for a finite element discretization of the Laplacian. The stencil of the Laplacian in 3 dimensions using trilinear cubic finite elements is given by

$$\frac{4}{3}\begin{bmatrix} -4 & -8 & -4 \\ -8 & & -8 \\ -4 & -8 & -4 \end{bmatrix} \quad \begin{bmatrix} -8 & & -8 \\ & 128 & \\ -8 & & -8 \end{bmatrix} \quad \begin{bmatrix} -4 & -8 & -4 \\ -8 & & -8 \\ -4 & -8 & -4 \end{bmatrix}, \tag{36}$$

so the generating symbol is given by

$$f(x) = \frac{4}{3}\left(128 - 32\left(\cos(x_1)\cos(x_2) + \cos(x_1)\cos(x_3) + \cos(x_2)\cos(x_3) + \cos(x_1)\cos(x_2)\cos(x_3)\right)\right).$$

As in the 2-dimensional case only one ω is needed and the results are comparable. The results of the circulant case can be found in Table 14, those for the Toeplitz case can be found in Table 15.

5. Conclusion

Aggregation-based multigrid methods for circulant and Toeplitz matrices can be analyzed using the classical theory. The non-optimality of non-smoothed aggregation-based multigrid methods can be explained easily by the lack of fulfillment of (11) by the prolongation and restriction operator in that case. Guided by this observation sufficient conditions for an improvement of the grid transfer operators by application of the Richardson iteration can be derived, including the optimal choice of the parameter. The results carry over from aggregates of size 2^d to larger aggregates. In future works the optimality of other coarsening ratios and the non-constant coefficient case will be further investigated.

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