

Algebraic multilevel iteration methods and the best approximation to $1/x$ in the uniform norm

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ALGEBRAIC MULTILEVEL ITERATION METHODS AND THE BEST APPROXIMATION TO $1/x$ IN THE UNIFORM NORM

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ABSTRACT. In this note, we provide simple convergence analysis for the algebraic multilevel iteration methods [37, 51]. We consider two examples of AMLI methods with different polynomial acceleration. The first one is based on shifted and scaled Chebyshev polynomial and the other on the polynomial of best approximation to x^{-1} on a finite interval $[\lambda_{\min}, \lambda_{\max}]$, $0 < \lambda_{\min} < \lambda_{\max}$ in the $\|\cdot\|_{\infty}$ norm. The construction of the latter polynomial is of interest by itself, and we have included a derivation of a recurrence relation for computing this polynomial. We have also derived several inequalities related to the error of best approximation, which we applied in the AMLI analysis.

1. INTRODUCTION

Nowadays, algebraic multigrid and multilevel methods provide powerful solution tools for a wide range of sparse matrix problems in science and engineering. The classical algebraic multigrid (AMG) algorithm was originally proposed in the early eighties [13, 14, 15]. From a practical point of view its description in [46] has made a great impact. In the last decade there has been a revival of research in the field of classical AMG [22], element-based AMG [18, 26, 29], spectral AMG [21], AMG based on energy-minimizing interpolation and smoothed aggregation [38, 48, 49, 52, 54], bootstrap AMG [16], adaptive smoothed aggregation [19] and adaptive algebraic multigrid [20]. While AMG methods can be viewed as matrix-based multigrid, there exist also various multilevel (ML) methods that utilize a sequence of coarse-grid operators that arise from rediscrretization of the continuous problem—based on its variational formulation—or from hierarchical basis transformation of the discrete problem. Multilevel methods evolved from two-level methods that have been introduced and analyzed for finite element elliptic systems in [4, 11]. For sharp two-sided bounds on the convergence rate of two-level methods see [57]. A straightforward recursive extension of the two-level methods leads to the class of hierarchical basis (HB) methods for which the condition number of the preconditioned system in general grows exponentially with the number of levels, cf. [56]. That is why one often combines HB methods with certain stabilization techniques [50]. By using specially constructed matrix polynomials HB-ML methods can be made optimal. Known as (linear) algebraic multilevel iteration (AMLI) such methods have been introduced in the late eighties [7, 8], for nonlinear AMLI methods see also [5, 6, 32]. Recent works on algebraic multilevel preconditioning methods mainly focus on additive and parameter-free methods [9, 32, 40], aggregation-based preconditioners [12, 36, 42], and on extending their theoretic foundation and their applicability to various nonconforming and discontinuous Galerkin (DG) discretizations of highly ill-conditioned problems [2, 10, 17, 23, 24, 25, 34, 35].

Such problems arise for example in continuum mechanics when highly heterogeneous or porous media such as human bone tissue or geocomposites are considered, which have a complicated hierarchical structure with multiple characteristic length scales. In [33] preliminary results are shown on the construction of robust two-level methods for elliptic problems with extremely rough coefficients.

The combination of AMLI and AMG techniques is a promising approach in view of increasing the robustness of multilevel solvers for this kind of applications. For instance it is known that standard AMG with piecewise constant interpolation yields an unstable multilevel method in general even though the related two-level method is stable, see, e.g., [51]. In such cases polynomial acceleration is a key tool for stabilizing the multilevel solution method.

A theoretical comparison of algebraic multigrid and multilevel methods can be found in [41]. A common framework for their analysis has been established in form of the abstract theory of subspace correction methods [53, 55]. A comprehensive exposition and analysis of various multilevel block factorization preconditioners, including AMG, has been presented in [51].

In this work we review the basic construction of multilevel methods as recursive extensions of two-level methods and consider polynomial acceleration techniques that can be employed in AMLI and AMG methods. In particular, we study the polynomial of best approximation to $1/x$ in uniform norm, derive recurrence relations and error estimates and show how these enter the convergence analysis and condition number bounds of the accelerated multilevel methods.

2. TWO-LEVEL AND MULTILEVEL METHODS

In this section we consider a two-level iterative method for the solution of a system of linear algebraic equations

$$(2.1) \quad A\mathbf{x} = \mathbf{b},$$

where $A \in \mathbb{R}^{N \times N}$, is symmetric and positive definite, $\mathbf{b} \in \mathbb{R}^N$ is a given right hand side. To describe a general two-level or multilevel multiplicative method, we denote $V = \mathbb{R}^N$, and also introduce a coarse space V_H , $V_H \subset V$, $N_H = \dim V_H$, $N_H < N$. In the following we will always assume that $V_H = \text{range}(P)$, where $P : \mathbb{R}^{N_H} \mapsto V$ and its matrix representation in the canonical basis of \mathbb{R}^{N_H} is given by the coefficients in the expansion of the basis in V_H via the basis in V . Clearly P is a full rank operator, and its matrix representation is oftentimes called *prolongation* or *interpolation* matrix.

2.1. Exact and inexact two-level methods and polynomial acceleration. We now consider a classical two-level preconditioning iteration, which utilizes a multiplicative preconditioner $B^{-1} \approx A^{-1}$.

Algorithm 2.1. Given $\mathbf{x} \in V$ the action $B^{-1}\mathbf{x}$ is defined via the following three steps:

1. Pre-smoothing: $\mathbf{y} = M^{-1}\mathbf{x}$.
2. Coarse grid correction: $\mathbf{z} = \mathbf{y} + P\tilde{B}_H^{-1}P^T(\mathbf{x} - A\mathbf{y})$.
3. Post-smoothing: $B^{-1}\mathbf{x} := \mathbf{z} + M^{-T}(\mathbf{x} - A\mathbf{z})$.

To apply this algorithm, for example in the Preconditioned Conjugate Gradient (PCG) method, one needs to define an appropriate smoother M and a coarse grid preconditioner \tilde{B}_H . The coarse grid preconditioner is an approximation to the restriction of A on V_H . This

restriction we denote by A_H and we have $A_H = P^T A P$ and $\tilde{B}_H^{-1} \approx A_H^{-1}$. To write down the closed form of B^{-1} we also need the symmetrization of M , denoted here with \bar{M} . This symmetrization is defined in a usual manner, namely \bar{M} satisfies

$$(I - \bar{M}^{-1}A) = (I - M^{-T}A)(I - M^{-1}A).$$

A simple calculation then shows that

$$(2.2) \quad \bar{M} = M(M + M^T - A)^{-1}M^T, \quad \text{and} \quad \bar{M}^{-1} = M^{-1} + M^{-T} - M^{-T}AM^{-1}.$$

Writing the three steps in the two-level algorithm in terms of \mathbf{x} then leads to

$$\begin{aligned} \mathbf{z} &= \left[M^{-1}\mathbf{x} + P\tilde{B}_H^{-1}P^T(\mathbf{x} - AM^{-1}\mathbf{x}) \right] \\ &= \left[M^{-1} + P\tilde{B}_H^{-1}P^T(I - AM^{-1}) \right] \mathbf{x}, \end{aligned}$$

and hence

$$\begin{aligned} B^{-1}\mathbf{x} &= \mathbf{z} + M^{-T}(\mathbf{x} - A\mathbf{z}) = M^{-T}\mathbf{x} + (I - M^{-T}A)\mathbf{z} \\ &= M^{-T}\mathbf{x} + (I - M^{-T}A) \left[M^{-1} + P\tilde{B}_H^{-1}P^T(I - AM^{-1}) \right] \mathbf{x} \\ &= M^{-T}\mathbf{x} + (I - M^{-T}A)M^{-1}\mathbf{x} \\ &\quad + (I - M^{-T}A)P\tilde{B}_H^{-1}P^T(I - AM^{-1})\mathbf{x} \\ &= \left[\bar{M}^{-1} + (I - M^{-T}A)P\tilde{B}_H^{-1}P^T(I - AM^{-1}) \right] \mathbf{x}. \end{aligned}$$

Since this identity holds for all $\mathbf{x} \in V$ we have that

$$(2.3) \quad B^{-1} = \bar{M}^{-1} + (I - M^{-T}A)P\tilde{B}_H^{-1}P^T(I - AM^{-1}).$$

The aim is to construct B such that the condition number $B^{-1}A$ is constant (independent of the size of A). We will always assume that the action of M^{-1} requires $\mathcal{O}(N)$ operations.

We distinguish two cases in choosing \tilde{B}_H :

$$(2.4) \quad \textit{exact} \text{ two level method if } \tilde{B}_H = A_H, \text{ where } A_H = P^T A P.$$

$$(2.5) \quad \textit{inexact} \text{ two level method if } \tilde{B}_H \neq A_H.$$

The exact two-level method is easier to analyze, in many cases has a uniformly bounded condition number, but is in general not practical, since N_H is usually taken proportional to N , and typical cases are $N_H = N/2$, $N_H = N/4$ or $N_H = N/8$. Then the size of the coarse level problem is comparable to the size of the original problem and hence the application of B^{-1} would require the solution of a coarse level problem which is of the same difficulty as the solution of (2.1).

On the other hand, in a typical inexact method the action \tilde{B}_H^{-1} is defined recursively, by the same algorithm. Clearly, in such case, computing the action of B^{-1} on a vector requires $\mathcal{O}(N)$ operations. Such method is known as multilevel V-cycle preconditioner. If in addition the condition number of $B^{-1}A$ is uniformly bounded, then we have an optimal method. However, depending on the choice of the coarse spaces V_H in the recursive application of the algorithm, one may also end up with a method for which this condition number depends on the size of the problem N . Here coarse spaces is in plural, since recursive application of Algorithm 2.1 requires more than one V_H . A typical example for such behavior is when A results from finite element discretization of a second order elliptic equation with conforming linear elements and

the coarse spaces V_H are chosen to interpolate piece-wise constant functions. In such cases one definitely wants to further improve the method by modifying \tilde{B}_H , without changing the coarse spaces.

In our focus will be the Algebraic Multi-Level Iteration (AMLI) methods, which are constructed as follows: Suppose that we have an *initial* coarse level preconditioner B_H . This means basically that we have in hand a B_H , and as an initial algorithm we consider Algorithm 2.1 with B_H instead of \tilde{B}_H . We would like to design now a \tilde{B}_H , in such a way that the inexact method becomes close to the exact two-level method. In doing this, we would like to keep the number of operations in calculating the action of B^{-1} under control, and also to decrease the condition number of $B^{-1}A$.

In AMLI for a given initial B_H the coarse-level preconditioner $\tilde{B}_H = B_{H,\nu}^{-1}$, is defined as

$$(2.6) \quad B_{H,\nu}^{-1} := q_{\nu-1}(B_H^{-1}A_H)B_H^{-1},$$

where $q_{\nu-1} \in \mathcal{P}_{\nu-1}$ is an appropriately chosen polynomial of degree less than or equal to $(\nu - 1)$ for some $\nu \geq 1$. To give a motivation for doing this, we list here three examples, which may be not practical, but are instructive:

- Set $\nu = 1$ and $q_0(x) = 1$, which results in $\tilde{B}_H = B_H$, that is we have no change in the preconditioner.
- Set $\nu = N_H$ and for a given non-singular operator $X_H : V_H \mapsto V_H$, define $q_{N_H-1}(X_H) = X_H^{-1}$. This results in the exact two-level method. Note that regardless of what form the initial coarse level preconditioner $B_H : V_H \mapsto V_H$ takes, as long as B_H is invertible the resulting method will be the exact two-level method.
- Again, let $\nu = N_H$ and in the notation of Algorithm 2.1, $\mathbf{r}_H = P^T(\mathbf{b} - A\mathbf{x})$. Let $q_{N_H-1}(X_H)$ be any polynomial such that

$$q_{N_H-1}(X_H)r_H = X_H^{-1}r_H.$$

As a result we get that $B_{H,\nu}^{-1}\mathbf{r}_H = A_H^{-1}r_H$, but the action of $B_{H,\nu}^{-1}$ depends on the argument, and hence we have a nonlinear preconditioner. For a given \mathbf{r}_H , such a polynomial $q_{\nu-1}(X_H)r_H$ can be constructed by applying $(\nu - 1)$ Preconditioned Conjugate Gradient iterations to the solution of

$$A_H\mathbf{e}_H = \mathbf{r}_H, \quad \text{with preconditioner } B_H^{-1}.$$

For $\nu = N_H$ as we have in this example, we immediately obtain the exact two level method. Since applying $(N_H - 1)$ PCG iterations may be expensive, one may take a fixed number of PCG iterations, namely $\nu = \mathcal{O}(1)$ and the resulting method is known as nonlinear AMLI method. More details about nonlinear AMLI methods are found in [32].

2.2. Error propagation operators and polynomial acceleration. The two-level multiplicative preconditioner B^{-1} constructed in the previous section may also be used as an *iterator*. A two-level iterative method generates a sequence of iterates $\mathbf{x}_{(i)}$ (for a given initial guess $\mathbf{x}_{(0)}$) via

$$(2.7) \quad \mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + B^{-1}\mathbf{r}_{(i)} = \mathbf{x}_{(i)} + B^{-1}(\mathbf{b} - A\mathbf{x}_{(i)}), \quad i = 0, 1, \dots$$

If \mathbf{x}_* is the exact solution to (2.1) and $\mathbf{e}_{(i)} = \mathbf{x}_* - \mathbf{x}_{(i)}$ is the error, then the *error propagation* operator E of the two-level iterative method (2.7) is written as

$$(2.8) \quad \mathbf{e}_{(i+1)} = E\mathbf{e}_{(i)}, \quad E = I - B^{-1}A.$$

As we pointed out, an inexact two-level method is based on approximating the coarse grid correction for the exact two level method

$$\mathbf{e}_H = A_H^{-1} r_H, \quad \text{with } r_H = P^T \mathbf{r}_{(i)}.$$

Hence the error transfer operator for one coarse-level update $\mathbf{x}_{(i)} + PB_H^{-1}P^T \mathbf{r}_{(i)}$ is given by

$$(2.9) \quad E_H = I - PB_H^{-1}P^T A$$

where B_H^{-1} is the inverse of the initial preconditioner (the approximation to A_H^{-1}) at the coarse level, which is used to build \tilde{B}_H .

The following simple identity will be useful in deriving the error propagation relation between the coarse and the fine-grid level.

Lemma 2.2. *Let $p_\nu(x) = 1 - q_{\nu-1}(x)x$. Then the following identity holds for the error propagation operator $E = I - B^{-1}A$, where B^{-1} is defined in Algorithm 2.1 with $\tilde{B}_H^{-1} = B_{H,\nu}^{-1}$:*

$$(2.10) \quad I - B^{-1}A = (I - M^{-T}A) \tilde{p}_\nu(E_H) (I - M^{-1}A)$$

where

$$(2.11) \quad \tilde{p}_\nu(x) := p_\nu(1 - x).$$

Proof. Let q_r be a polynomial of degree less or equal to r and $A_H = P^T A P$ denote the coarse-grid matrix. We will first prove that

$$(2.12) \quad P q_r(B_H^{-1}A_H) B_H^{-1}P^T A = q_r(PB_H^{-1}P^T A) PB_H^{-1}P^T A.$$

It suffices to prove the identity (2.12) for the case $q_r(x) = x^k$, $k \leq r$. For $k = 0$ the result is obvious. For $k = 1$ we obtain

$$PB_H^{-1}A_H B_H^{-1}P^T A = PB_H^{-1}P^T A P B_H^{-1}P^T A,$$

which is true since $A_H = P^T A P$. Finally, assuming that (2.12) holds true for $k = j - 1$ we have

$$(2.13) \quad \begin{aligned} P (B_H^{-1}A_H)^j B_H^{-1}P^T A &= P (B_H^{-1}A_H)^{j-1} B_H^{-1}P^T A P B_H^{-1}P^T A \\ &= (PB_H^{-1}P^T A)^{j-1} PB_H^{-1}P^T A P B_H^{-1}P^T A \\ &= (PB_H^{-1}P^T A)^j PB_H^{-1}P^T A. \end{aligned}$$

Using (2.3) we find

$$(2.14) \quad \begin{aligned} I - B^{-1}A &= I - \bar{M}^{-1}A - (I - M^{-T}A) PB_{H,\nu}^{-1}P^T (I - AM^{-1}) A \\ &= (I - M^{-T}A) (I - M^{-1}A) \\ &\quad - (I - M^{-T}A) PB_{H,\nu}^{-1}P^T A (I - M^{-1}A) \\ &= (I - M^{-T}A) (I - PB_{H,\nu}^{-1}P^T A) (I - M^{-1}A). \end{aligned}$$

Moreover, since $p_\nu(x) = 1 - q_{\nu-1}(x)x$ we can rewrite (2.6) in the form

$$(2.15) \quad \begin{aligned} B_{H,\nu}^{-1} &= (I - p_\nu(B_H^{-1}A_H)) A_H^{-1} \\ &= (I - (I - q_{\nu-1}(B_H^{-1}A_H)) B_H^{-1}A_H) A_H^{-1} \\ &= q_{\nu-1}(B_H^{-1}A_H) B_H^{-1}. \end{aligned}$$

Then by substituting (2.15) in (2.14) and using (2.13) and finally (2.9) we obtain the following representation of (2.8):

$$\begin{aligned}
I - B^{-1}A &= (I - M^{-T}A)(I - Pq_{\nu-1}(B_H^{-1}A_H)B_H^{-1}P^T A)(I - M^{-1}A) \\
&= (I - M^{-T}A)(I - q_{\nu-1}(PB_H^{-1}P^T A)PB_H^{-1}P^T A)(I - M^{-1}A) \\
&= (I - M^{-T}A)(I - q_{\nu-1}(I - E_H)(I - E_H))(I - M^{-1}A) \\
&= (I - M^{-T}A)(p_\nu(I - E_H))(I - M^{-1}A) \\
(2.16) \quad &= (I - M^{-T}A)\tilde{p}_\nu(E_H)(I - M^{-1}A)
\end{aligned}$$

□

We move on to describe the multilevel case and prove a condition number estimate, which depends on the approximation properties of V_H as well as on the estimates involving $q_{\nu-1}(\cdot)$.

2.3. The algebraic multilevel iteration (AMLI) algorithm. We now focus on more implementation and analysis details for multilevel methods, which are obtained by recursively applying Algorithm 2.1. In what follows we will denote by $B^{(k)}$ a preconditioner for a finite element (stiffness) matrix $A^{(k)}$ corresponding to a k times refined mesh ($0 \leq k \leq \ell$). We will also make use of the corresponding k -th level hierarchical matrix $\tilde{A}^{(k)}$, which is related to $A^{(k)}$ via a two-level hierarchical basis (HB) transformation $J^{(k)}$, i.e.,

$$(2.17) \quad \tilde{A}^{(k)} = (J^{(k)})^T A^{(k)} J^{(k)}.$$

By $A_{ij}^{(k)}$ and $\tilde{A}_{ij}^{(k)}$, $1 \leq i, j \leq 2$, we denote the blocks of $A^{(k)}$ and $\tilde{A}^{(k)}$ that correspond to the fine-coarse partitioning of degrees of freedom (DOF) where the DOF associated with the coarse mesh are numbered last.

The aim is to build a multilevel preconditioner $B^{(\ell)}$ for the coefficient matrix $A^{(\ell)} := A_h$ at the level of the finest mesh that has a uniformly bounded (relative) condition number

$$\kappa(B^{(\ell)-1}A^{(\ell)}) = \mathcal{O}(1),$$

and an optimal computational complexity, that is, linear in the number of degrees of freedom N_ℓ at the finest mesh (grid). In order to achieve this goal hierarchical basis methods can be combined with various types of stabilization techniques.

One particular purely algebraic stabilization technique is the so-called Algebraic Multi-Level Iteration (AMLI) method, where a specially constructed matrix polynomial $p^{(k)}$ of degree ν_k is employed at some or at all levels $k = k_0 + 1, \dots, \ell$. The AMLI methods have originally been introduced and studied in a multiplicative form, see [7, 8]. The presentation in this section follows Reference [32].

Starting at level 0 (associated with the coarsest mesh) on which a complete LU factorization of the matrix $A^{(0)}$ is performed, we define

$$(2.18) \quad B^{(0)} := A^{(0)}.$$

Given the preconditioner $B^{(k-1)}$ at level $k-1$ the preconditioner $B^{(k)}$ at level k is defined by

$$(2.19) \quad B^{(k)} := L^{(k)}D^{(k)}U^{(k)}$$

where

$$(2.20) \quad L^{(k)} := \begin{bmatrix} I & 0 \\ \tilde{A}_{21}^{(k)} C_{11}^{(k)-1} & I \end{bmatrix}, \quad U^{(k)} := \begin{bmatrix} I & C_{11}^{(k)-1} \tilde{A}_{12}^{(k)} \\ 0 & I \end{bmatrix},$$

and

$$(2.21) \quad D^{(k)} := \begin{bmatrix} C_{11}^{(k)} & 0 \\ 0 & Z^{(k-1)} \end{bmatrix}.$$

Here we use the approximation

$$(2.22) \quad Z^{(k-1)} := A^{(k-1)} \left(I - p^{(k)}(B^{(k-1)})^{-1} A^{(k-1)} \right)^{-1}$$

to the Schur complement $S = A^{(k-1)} - \tilde{A}_{21}^{(k)} C_{11}^{(k)-1} \tilde{A}_{12}^{(k)}$ where $A^{(k-1)} := A_H = \tilde{A}_{22}^{(k)}$ is the coarse-level stiffness matrix (stiffness matrix at level $k-1$), which can be obtained from the two-level hierarchical basis representation

$$(2.23) \quad \tilde{A}^{(k)} = \begin{bmatrix} \tilde{A}_{11}^{(k)} & \tilde{A}_{12}^{(k)} \\ \tilde{A}_{21}^{(k)} & \tilde{A}_{22}^{(k)} \end{bmatrix} = \begin{bmatrix} A_{11}^{(k)} & \tilde{A}_{12}^{(k)} \\ \tilde{A}_{21}^{(k)} & A^{(k-1)} \end{bmatrix}$$

at level k , and $p^{(k)}$ is a polynomial of degree ν_k satisfying

$$(2.24) \quad p^{(k)}(0) = 1.$$

It is easily seen that (2.22) is equivalent to

$$(2.25) \quad Z^{(k-1)-1} = B^{(k-1)-1} q^{(k)}(A^{(k-1)} B^{(k-1)-1})$$

where the polynomial $q^{(k)}$ is given by

$$(2.26) \quad q^{(k)}(x) = \frac{1 - p^{(k)}(x)}{x}.$$

We note that the multilevel preconditioner defined via (2.19) is getting close to a two-level method when $q^{(k)}(x)$ approximates well $\frac{1}{x}$ in which case $Z^{(k-1)-1} \approx A^{(k-1)-1}$. In order to construct an efficient multilevel method the action of $Z^{(k-1)-1}$ on an arbitrary vector should be much cheaper to compute (in terms of the number of arithmetic operations) than the action of $A^{(k-1)-1}$. Optimal order solution algorithms typically require that the arithmetic work for one application of $Z^{(k-1)-1}$ is of the order $\mathcal{O}(N_{k-1})$ where N_{k-1} denotes the number of unknowns at level $k-1$.

A linear system with $B^{(k)}$, an unknown vector $\mathbf{v}^{(k)} = (\mathbf{v}_1^{(k)T}, \mathbf{v}_2^{(k)T})^T$, and right hand side vector $\mathbf{d}^{(k)} = (\mathbf{d}_1^{(k)T}, \mathbf{d}_2^{(k)T})^T$ at level k can be written as

$$\begin{bmatrix} C_{11}^{(k)} & 0 \\ \tilde{A}_{21}^{(k)} & Z^{(k-1)} \end{bmatrix} \begin{bmatrix} I & C_{11}^{(k)-1} \tilde{A}_{12}^{(k)} \\ 0 & I \end{bmatrix} \begin{pmatrix} \mathbf{v}_1^{(k)} \\ \mathbf{v}_2^{(k)} \end{pmatrix} = \begin{pmatrix} \mathbf{d}_1^{(k)} \\ \mathbf{d}_2^{(k)} \end{pmatrix}.$$

Its solution involves the solution of a system

$$B^{(k-1)} \mathbf{v}^{(k-1)} = \mathbf{d}^{(k-1)}$$

at level $(k-1)$ for some right hand side $\mathbf{d}^{(k-1)}$. Let

$$\mathbf{u}^{(k)} = \begin{pmatrix} \mathbf{u}_1^{(k)} \\ \mathbf{u}_2^{(k)} \end{pmatrix} = \begin{bmatrix} I & C_{11}^{(k)-1} \tilde{A}_{12}^{(k)} \\ 0 & I \end{bmatrix} \begin{pmatrix} \mathbf{v}_1^{(k)} \\ \mathbf{v}_2^{(k)} \end{pmatrix},$$

then we have

$$(2.27) \quad \begin{aligned} \mathbf{u}_1^{(k)} &= C_{11}^{(k)-1} \mathbf{d}_1^{(k)} \\ Z^{(k-1)} \mathbf{u}_2^{(k)} &= \mathbf{d}_2^{(k)} - \tilde{A}_{21}^{(k)} \mathbf{u}_1^{(k)} =: \mathbf{w}^{(k-1)}. \end{aligned}$$

Using (2.25) we write (2.27) in the form

$$(2.28) \quad B^{(k-1)} \mathbf{u}_2^{(k)} = q^{(k)}(A^{(k-1)} B^{(k-1)-1}) \mathbf{w}^{(k-1)}$$

where $q^{(k)}(x) = \frac{1-p^{(k)}(x)}{x} = a_0^{(k)} + a_1^{(k)}x + \dots + a_{\nu_k-1}^{(k)}x^{\nu_k-1}$. Hence

$$\begin{aligned} \mathbf{d}^{(k-1)} &= q^{(k)}(A^{(k-1)} B^{(k-1)-1}) \mathbf{w}^{(k-1)}, \\ \mathbf{v}^{(k-1)} &= \mathbf{u}_2^{(k)}. \end{aligned}$$

The following algorithm computes the solution of

$$(2.29) \quad B^{(\ell)} \mathbf{v}^{(\ell)} = \mathbf{d}^{(\ell)}.$$

Algorithm 2.3. [Linear AMLI] (cf., [8])

$$(2.30) \quad \begin{aligned} &\text{for } k = 1 \text{ to } \ell \text{ set } \sigma_k := 0 \\ &k := \ell \\ \text{forward:} & \quad \sigma_k := \sigma_k + 1 \\ & \quad \text{if } \sigma_k = 1 \\ & \quad \quad \mathbf{d}^{(k)} := (J^{(k)})^T \mathbf{d}^{(k)} \\ & \quad \quad \mathbf{v}_1^{(k)} := (C_{11}^{(k)})^{-1} \mathbf{d}_1^{(k)} \\ & \quad \quad \mathbf{w}^{(k-1)} := \mathbf{d}_2^{(k)} - \tilde{A}_{21}^{(k)} \mathbf{v}_1^{(k)} \\ & \quad \quad \mathbf{d}^{(k-1)} := a_{\nu_k-1}^{(k)} \mathbf{w}^{(k-1)} \\ & \quad \text{else} \\ & \quad \quad \mathbf{d}^{(k-1)} := A^{(k-1)} \mathbf{v}^{(k-1)} + a_{\nu_k-\sigma_k}^{(k)} \mathbf{d}^{(k-1)} \\ & \quad \text{end} \\ & \quad k := k - 1 \\ & \quad \text{if } k > 0 \text{ goto forward} \\ & \quad \text{solve } A^{(0)} \mathbf{v}^{(0)} = \mathbf{d}^{(0)} \text{ for } \mathbf{v}^{(0)} \end{aligned}$$

$$(2.32) \quad \begin{aligned} \text{backward:} & \quad k := k + 1 \\ & \quad \mathbf{v}_2^{(k)} := \mathbf{v}^{(k-1)} \\ & \quad \text{if } \sigma_k < \nu_k \text{ goto forward} \\ & \quad \quad \mathbf{v}_1^{(k)} := \mathbf{v}_1^{(k)} - (C_{11}^{(k)})^{-1} \tilde{A}_{12}^{(k)} \mathbf{v}_2^{(k)} \\ & \quad \quad \mathbf{v}^{(k)} := J^{(k)} \mathbf{v}^{(k)} \end{aligned}$$

$$(2.33) \quad \begin{aligned} &\sigma_k := 0 \\ &\text{if } k < \ell \text{ goto backward} \end{aligned}$$

Here the vector $\boldsymbol{\nu} = (\nu_1, \nu_2, \dots, \nu_\ell)^T$ defines the cycle, i.e., $\nu_k = 1$ for $1 \leq k \leq \ell$ corresponds to the V-cycle, and $\nu_k = 2$ for $1 \leq k < \ell$, $\nu_\ell = 1$, corresponds to the classical W-cycle. Higher-order stabilization or mixed cycles with varying polynomial degree are possible and sometimes preferable from a computational point of view.

Algorithm (2.3) is based on the multiplicative two-level preconditioner

$$(2.34) \quad C^{(k)} = \begin{bmatrix} C_{11}^{(k)} & \tilde{A}_{12}^{(k)} \\ \tilde{A}_{21}^{(k)} & A^{(k-1)} + \tilde{A}_{21}^{(k)}(C_{11}^{(k)})^{-1}\tilde{A}_{12}^{(k)} \end{bmatrix}.$$

It uses the approximations $C_{11}^{(k)-1}$ for $A_{11}^{(k)-1}$, and $Z^{(k-1)-1}$ for the inverse of the Schur complement at level k , see (2.25). The action of the matrix polynomial $q^{(k)}(A^{(k-1)}B^{(k-1)})^{-1}$ in (2.25) on a vector is computed via Horner's rule, where the coefficients of $q^{(k)}(x)$ are given by $a_{\nu_k - \sigma_k}^{(k)}$, $1 \leq \sigma_k \leq \nu_k$.

The matrices $\tilde{A}_{12}^{(k)}$ and $\tilde{A}_{21}^{(k)}$ are the off-diagonal blocks of the two-level hierarchical basis matrix $\tilde{A}^{(k)}$ at level k , and $A^{(k-1)}$ is the matrix associated with the coarse grid (with respect to the coarse-grid nodal basis).

2.4. Condition number estimates. Let us now study the spectral condition number $\kappa(B^{(\ell)-1}A^{(\ell)})$ where $B^{(\ell)}$ denotes the recursively defined linear AMLI preconditioner, cf. (2.18)–(2.22). The presented results are in the spirit of [3, 7, 8] and have the same recursive structure, that is, an estimate at level k involves the same type of estimate at level $k - 1$.

The basic assumption in the analysis of the multilevel preconditioner is an approximation property of the form

$$(2.35) \quad \theta_0^{(k)} \boldsymbol{v}^T A^{(k)} \boldsymbol{v} \leq \boldsymbol{v}^T C^{(k)} \boldsymbol{v} \leq \theta_1^{(k)} \boldsymbol{v}^T A^{(k)} \boldsymbol{v} \quad \forall \boldsymbol{v}, \quad k = 1, 2, \dots, \ell.$$

Additionally, it reasonable to assume that

$$(2.36) \quad 0 < \theta_0 < \theta_0^{(k)} \leq \theta_1^{(k)} < \theta_1 < \infty, \quad 1 \leq k \leq \ell.$$

The following lemma shows the basic induction step in the multilevel analysis.

Lemma 2.4. *If the multilevel preconditioner at level $j = k - 1$ satisfies the relation*

$$(2.37) \quad \rho_0^{(j)} \boldsymbol{v}^T A^{(j)} \boldsymbol{v} \leq \boldsymbol{v}^T B^{(j)} \boldsymbol{v} \leq \rho_1^{(j)} \boldsymbol{v}^T A^{(j)} \boldsymbol{v} \quad \forall \boldsymbol{v}$$

then the preconditioner at level $j = k$ satisfies the same relation with the constants

$$(2.38a) \quad \rho_0^{(k)} = \frac{\theta_0^{(k)}}{\max\{1, r_1^{(k-1)}\}},$$

$$(2.38b) \quad \rho_1^{(k)} = \frac{\theta_1^{(k)}}{\min\{1, r_0^{(k-1)}\}},$$

where

$$(2.39a) \quad r_0^{(k-1)} = \min_{x \in I_\sigma^{(k-1)}} x q^{(k)}(x),$$

$$(2.39b) \quad r_1^{(k-1)} = \max_{x \in I_\sigma^{(k-1)}} x q^{(k)}(x),$$

and $q^{(k)}$ can be any polynomial that satisfies $q^{(k)}(x) \geq 0 \quad \forall x \in I_\sigma^{(k-1)} = [1/\rho_1^{(k-1)}, 1/\rho_0^{(k-1)}]$.

Proof. In order to prove the transition from level $k - 1$ to level k we consider the matrix (2.34) corresponding to the multiplicative two-level preconditioner at level k , which can be factored as

$$C^{(k)} = L^{(k)} \bar{D}^{(k)} L^{(k)T}$$

where

$$\bar{D}^{(k)} = \begin{bmatrix} C_{11}^{(k)} & 0 \\ 0 & A^{(k-1)} \end{bmatrix}$$

and the matrix $L^{(k)}$ is given by (2.20). Now from (2.25) we see that for any vector $\mathbf{y}_2 \neq \mathbf{0}$ and $\mathbf{x}_2 := (A^{(k-1)})^{-1/2} \mathbf{y}_2$ we have

$$\begin{aligned} & \frac{\mathbf{y}_2^T (Z^{(k-1)})^{-1} \mathbf{y}_2}{\mathbf{y}_2^T (A^{(k-1)})^{-1} \mathbf{y}_2} \\ & \frac{\mathbf{y}_2^T B^{(k-1)-1} q^{(k)} (A^{(k-1)} B^{(k-1)-1}) \mathbf{y}_2}{\mathbf{y}_2^T (A^{(k-1)})^{-1} \mathbf{y}_2} \\ = & \frac{\mathbf{x}_2^T (A^{(k-1)})^{1/2} B^{(k-1)-1} q^{(k)} (A^{(k-1)} B^{(k-1)-1}) (A^{(k-1)})^{1/2} \mathbf{x}_2}{\mathbf{x}_2^T \mathbf{x}_2} \\ = & \frac{\mathbf{x}_2^T X q^{(k)}(X) \mathbf{x}_2}{\mathbf{x}_2^T \mathbf{x}_2} \end{aligned}$$

where $X = (A^{(k-1)})^{1/2} B^{(k-1)-1} (A^{(k-1)})^{1/2}$ and thus the relation

$$(2.40) \quad r_0^{(k-1)} \mathbf{y}_2^T Z^{(k-1)} \mathbf{y}_2 \leq \mathbf{y}_2^T A^{(k-1)} \mathbf{y}_2 \leq r_1^{(k-1)} \mathbf{y}_2^T Z^{(k-1)} \mathbf{y}_2$$

holds with constants $r_0^{(k-1)}$ and $r_1^{(k-1)}$ defined in (2.39). Further,

$$(2.41) \quad \frac{\mathbf{v}^T C^{(k)} \mathbf{v}}{\mathbf{v}^T B^{(k)} \mathbf{v}} = \frac{\mathbf{y}^T \bar{D}^{(k)} \mathbf{y}}{\mathbf{y}^T D^{(k)} \mathbf{y}} = \frac{\mathbf{y}_1^T C_{11}^{(k)} \mathbf{y}_1 + \mathbf{y}_2^T A^{(k-1)} \mathbf{y}_2}{\mathbf{y}_1^T C_{11}^{(k)} \mathbf{y}_1 + \mathbf{y}_2^T Z^{(k-1)} \mathbf{y}_2},$$

for all $\mathbf{v} \neq \mathbf{0}$ and $\mathbf{y} = (\mathbf{y}_1^T, \mathbf{y}_2^T)^T = L^{(k)} \mathbf{v}$ and thus, by using (2.40), we find that for all $\mathbf{v} \in V$,

$$(2.42) \quad \min\{1, r_0^{(k-1)}\} \mathbf{v}^T B^{(k)} \mathbf{v} \leq \mathbf{v}^T C^{(k)} \mathbf{v} \leq \max\{1, r_1^{(k-1)}\} \mathbf{v}^T B^{(k)} \mathbf{v},$$

Finally, we combine the estimates

$$(2.43) \quad \max_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T A^{(k)} \mathbf{v}}{\mathbf{v}^T B^{(k)} \mathbf{v}} \leq \max_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T A^{(k)} \mathbf{v}}{\mathbf{v}^T C^{(k)} \mathbf{v}} \max_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T C^{(k)} \mathbf{v}}{\mathbf{v}^T B^{(k)} \mathbf{v}},$$

and

$$(2.44) \quad \min_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T A^{(k)} \mathbf{v}}{\mathbf{v}^T C^{(k)} \mathbf{v}} \min_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T C^{(k)} \mathbf{v}}{\mathbf{v}^T B^{(k)} \mathbf{v}} \leq \min_{\mathbf{v} \neq \mathbf{0}} \frac{\mathbf{v}^T A^{(k)} \mathbf{v}}{\mathbf{v}^T B^{(k)} \mathbf{v}},$$

with (2.42) and (2.35) and for all $\mathbf{v} \in V$ we obtain

$$(2.45) \quad \frac{1}{\theta_1^{(k)}} \min\{1, r_0^{(k-1)}\} \mathbf{v}^T B^{(k)} \mathbf{v} \leq \mathbf{v}^T A^{(k)} \mathbf{v} \leq \frac{1}{\theta_0^{(k)}} \max\{1, r_1^{(k-1)}\} \mathbf{v}^T B^{(k)} \mathbf{v},$$

which proves the lemma. \square

The following theorem provides an estimate of the (relative) condition number of the multilevel preconditioner $B^{(\ell)}$.

Theorem 2.5. *Assume that the approximation property (2.35) is satisfied on all levels k , $1 \leq k \leq \ell$, which means that (2.36) is true for some positive constants θ_0 and θ_1 . Further, let $0 < \rho_0 < \rho_0^{(k-1)} \leq \rho_1^{(k-1)} < \rho_1 < \infty$ for all $k = 1, 2, \dots, \ell$. Then the estimate*

$$(2.46) \quad \kappa(B^{(\ell)-1}A^\ell) \leq \frac{\theta_1 \max\{1, r_1\}}{\theta_0 \min\{1, r_0\}}$$

holds where

$$(2.47a) \quad r_0 = \min_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q^{(k)}(x),$$

$$(2.47b) \quad r_1 = \max_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q^{(k)}(x).$$

The condition number $\kappa(B^{(\ell)-1}A^\ell)$ is uniformly bounded if

$$(2.48) \quad \frac{\theta_1 \max\{1, r_1\}}{\theta_0 \min\{1, r_0\}} \leq \frac{\rho_1}{\rho_0}.$$

Proof. Since $B^{(0)} = A^{(0)}$ implies $\lambda_{\min}(B^{(0)-1}A^{(0)}) = \lambda_{\max}(B^{(0)-1}A^{(0)}) = 1$ the bound (2.37) holds for $j = 0$ and $\rho_0^{(0)} = \rho_1^{(0)} = 1$. Then a repeated application of Lemma 2.4 finally results in the estimate (2.46) for the multilevel preconditioner $B^{(\ell)}$. Clearly this estimate does not depend on the number of levels ℓ if (2.48) holds. \square

3. BEST POLYNOMIAL APPROXIMATION TO $1/x$ IN UNIFORM NORM

In this section we prove a three term recurrence relation for the polynomials of best uniform approximation to $1/x$ on a finite interval. We use symbolic computation to derive and prove the recurrence relation. The specific form of these polynomials that we derive here is suitable for the AMLI analysis from the previous section and we provide such analysis in Section 4.

The polynomial of best approximation in uniform norm to $1/x$ on a finite interval has been known for some time and can be found in classical texts on approximation theory, for example, see [39, 45, 1]. The problem of approximating x^{-1} has also been considered by Chebyshev [47] more than 100 years ago. A more recent work on this topic, which we will use in the derivation of the recurrence relation is [28].

3.1. Notation. Our considerations are on a finite interval, $[\lambda_{\min}, \lambda_{\max}]$, with $0 < \lambda_{\min} < \lambda_{\max} < \infty$. Since our aim is to use the construction here for preconditioning of linear systems, we introduce the condition number $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}} > 1$, and

$$\sigma = \frac{1}{\lambda_{\max} - \lambda_{\min}}, \quad a = \frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} = \frac{\kappa + 1}{\kappa - 1}.$$

Note that $a > 1$ and $\sigma > 0$. The change of variables

$$t = \frac{2}{\lambda_{\max} - \lambda_{\min}} \left(x - \frac{\lambda_{\max} + \lambda_{\min}}{2} \right) = 2\sigma x - a,$$

maps the interval $[\lambda_{\max}, \lambda_{\min}]$ to $[-1, 1]$. The inverse map is

$$x = \frac{1}{2\sigma}(t + a), \quad \text{and} \quad \frac{1}{x} = \frac{2\sigma}{t + a}.$$

We thus aim to find the polynomial of degree less than or equal to m of best approximation in $\|\cdot\|_{\infty,[-1,1]}$ norm of $f(t) = \frac{1}{t+a}$, $a > 1$. We note that if $Q_m(t)$ is the polynomial of best approximation to $1/(t+a)$ on $[-1, 1]$, and the error of approximation is

$$E_{[-1,1]} = \min_{Q \in \mathcal{P}_m} \left\| \frac{1}{t+a} - Q \right\|_{\infty,[-1,1]},$$

then

$$(3.1) \quad q_m(x) := 2\sigma Q_m(2\sigma x - a), \quad \text{and} \quad E = \min_{q \in \mathcal{P}_m} \left\| \frac{1}{x} - q \right\|_{\infty, [\lambda_{\min}, \lambda_{\max}]} = 2\sigma E_{[-1,1]}.$$

are the polynomial of best approximation in $\|\cdot\|_{\infty}$ norm on $[\lambda_{\min}, \lambda_{\max}]$ and the error of approximation respectively.

We denote the Chebyshev polynomial of degree k by T_k . For $T_k(x) \in \mathcal{P}_k$. we have

$$T_k(\xi) = \frac{1}{2} \left[(\xi + \sqrt{\xi^2 - 1})^k + (\xi - \sqrt{\xi^2 - 1})^k \right] = \frac{1}{2} \left[(\xi + \sqrt{\xi^2 - 1})^k + (\xi - \sqrt{\xi^2 - 1})^k \right].$$

We recall that

$$T_k(t) = \cos k \arccos(t), \quad t \in [-1, 1].$$

and denote

$$(3.2) \quad \delta := a - \sqrt{a^2 - 1} = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}, \quad \eta = -\delta$$

Observe that δ is the CG-convergence rate estimate, when λ_{\max} and λ_{\min} are the extreme eigenvalues of a positive definite matrix, (see, e.g. M. R. Hestenes and E. Stiefel [27]). Note also that $0 \leq \delta < 1$, $\delta^{-1} = a + \sqrt{a^2 - 1}$, $\eta < 0$ and $\delta = |\eta|$.

With this notation in hand, we have the following identities,

$$(3.3) \quad a = -\frac{1}{2}(\eta + \eta^{-1}), \quad \frac{1}{t+a} = \frac{2}{2t - \eta - \eta^{-1}},$$

and directly from the expression for $T_k(\xi)$ given above, we also have

$$(3.4) \quad T_k(a) = \frac{1}{2}(-1)^k(\eta^k + \eta^{-k}), \quad T_k(-a) = \frac{1}{2}(\eta^k + \eta^{-k}).$$

Next we give the best polynomial approximation to $\frac{1}{t+a}$ as it is given in [45] and [28].

Theorem 3.1. *Let $m \geq 1$ be a fixed integer. The polynomial $Q_m \in \mathcal{P}_m$, which furnishes the best approximation to $\frac{1}{t+a}$ in the L_{∞} norm on $[-1, 1]$ is*

$$Q_m(t) = -\frac{2}{\eta - \eta^{-1}} + \frac{4}{\eta - \eta^{-1}} \sum_{j=0}^{m-1} \eta^j T_j(x) - \frac{4\eta^{m-1}}{(\eta - \eta^{-1})^2} T_m(x).$$

The error of best approximation is

$$E_{[-1,1]} = \min_{Q \in \mathcal{P}_m} \left\| \frac{1}{t+a} - Q \right\|_{\infty,[-1,1]} = \frac{\delta^m}{a^2 - 1}.$$

Proof. See [45] or [28]. □

The following corollary is immediate and follows after a simple calculation.

Corollary 3.2. *If $E_{m, [\lambda_{\min}, \lambda_{\max}]}$ is the error of approximation with polynomial of degree m on the interval $[\lambda_{\min}, \lambda_{\max}]$, $0 < \lambda_{\min} < \lambda_{\max} < \infty$ then*

$$(3.5) \quad E_{m, [\lambda_{\min}, \lambda_{\max}]} = 2\delta^{m-1} E_{0, [\sqrt{\lambda_{\min}}, \sqrt{\lambda_{\max}}]}^2,$$

where $E_{0, [\sqrt{\lambda_{\min}}, \sqrt{\lambda_{\max}}]}$ is easily calculated to be

$$E_{0, [\sqrt{\lambda_{\min}}, \sqrt{\lambda_{\max}}]} = \frac{1}{2} \left(\frac{1}{\sqrt{\lambda_{\min}}} - \frac{1}{\sqrt{\lambda_{\max}}} \right).$$

For computations, the following result is useful, since it gives a straightforward way of computing the polynomial of best approximation. By means of algorithms for symbolic summation a simple closed form for the polynomial of best approximation stated above as well as a short recurrence relation can be found completely automatically. Nowadays there exist plenty of methods and implementations thereof that are up to complete these tasks [43]. It is in the nature of these algorithms that discovering new identities and relations means having a proof at hand at the same time.

For our specific problem we choose to apply the Mathematica package SumCracker developed and implemented by M. Kauers [31]. We are going to use two of the features of this package: discovering (thus proving) closed form representations, and discovering (thus proving) recurrence relations for admissible sequences. Admissibility in this context means that the input for this algorithm consists of expressions that satisfy systems of difference equations, i.e., recurrence relations, with polynomial coefficients. This is certainly the case for Chebyshev polynomials. Informally speaking, the admissible sequences are translated into a difference ring context. In this difference ring computations are carried out using known techniques for commutative, multivariate polynomial rings, especially Gröbner bases. The results of these computations can then be interpreted as statements about the original admissible sequences. For a detailed description of this and further algorithms contained in SumCracker we refer to [30, 31].

Theorem 3.3. *The best approximation out of \mathcal{P}_m to $\frac{1}{t+a}$ in the L_∞ norm on $[-1, 1]$ is*

$$Q_m(t) = \frac{1}{t+a} \left(1 - \frac{2\eta^m}{(\eta - \eta^{-1})^2} R_{m+1}(t) \right),$$

where

$$R_{m+1}(t) = \eta^{-1} T_{m+1}(t) - 2T_m(t) + \eta T_{m-1}(t).$$

Furthermore for the polynomials of best approximation the following three term recurrence relation holds:

$$(3.6) \quad \eta^{-1} Q_{m+2}(t) - 2t Q_{m+1}(t) + \eta Q_m(t) = -2, \quad m = 0, 1, \dots$$

with

$$Q_0(t) = \frac{a}{a^2 - 1}, \quad Q_1(t) = \frac{1}{\sqrt{a^2 - 1}} - \frac{t}{a^2 - 1}.$$

The error of approximation is:

$$E_{[-1,1]} = \min_{Q \in \mathcal{P}_m} \left\| \frac{1}{t+a} - Q \right\|_{\infty, [-1,1]} = \frac{\delta^m}{a^2 - 1}.$$

Proof. The closed form can be obtained in an instance by an application of SumCracker's command "Crack" as follows:

```
In[1]:= Crack[SUM[ηjChebyshevT[j, t], {j, 0, m - 1}]]
Out[1]= 
$$\frac{-\eta^{m+1}\text{ChebyshevT}[m + 1, t] + t^m(2\eta t - 1)\text{ChebyshevT}[m, t] - \eta t + 1}{\eta^2 - 2\eta t + 1}$$

```

From the sum representation given in Theorem 3.1 it is obvious that $Q_m(t)$ is indeed a polynomial of degree m . Certainly it is also an immediate consequence of the three term recurrence relation together with the initial values. This recurrence, however, can again be obtained completely automatic:

```
In[2]:= GetLinearRecurrence[Q[m, t], In → m, Head → Q]
Out[2]= 
$$Q[m + 2] == -2\eta - \eta^2 Q[m] + 2t\eta Q[m + 1]$$

```

Here $Q[m, t]$ was defined as the polynomial of best approximation, the option "In" specifies the discrete variable along which we look for a recurrence relation and the option "Head" declares which variable shall be used for a concise output. The default head would be "SUM". The initial values for the recurrence are easily computed as well, which completes the proof of the theorem. \square

Another proof of this theorem is given in the appendix.

The next lemma gives an estimate on $|R_{m+1}(t)|$ by a linear polynomial, which is used later to derive sufficient condition for the positivity of $q_m(\cdot)$.

Lemma 3.4. *The following estimate holds for the polynomial $R_{m+1}(t)$ defined in Theorem 3.3:*

$$(3.7) \quad -2(t + a) \leq R_{m+1}(t) \leq 2(t + a), \quad t \in [-1, 1].$$

Proof. Recall that by the definition of η and δ (see (3.2)), we have that $\eta < 0$, and $|\eta| = \delta$. Let $t = \cos \alpha$, for $\alpha \in [0, \pi]$. Then we find that

$$(3.8) \quad \begin{aligned} R_{m+1}(t) + 2t - \eta - \eta^{-1} &= \eta^{-1}(T_{m+1}(t) - 1) - 2(T_m(t) - t) + \eta(T_{m-1}(t) + 1) \\ &= -2\eta^{-1} \sin^2 \frac{m+1}{2} \alpha + 4 \sin \frac{m+1}{2} \alpha \sin \frac{m-1}{2} \alpha \\ &\quad - 2\eta \sin^2 \frac{m-1}{2} \alpha \\ &= -2\eta^{-1} \left(\sin \frac{m+1}{2} \alpha - \eta \sin \frac{m-1}{2} \alpha \right)^2 \end{aligned}$$

$$(3.9) \quad = 2\delta^{-1} \left(\sin \frac{m+1}{2} \alpha + \delta \sin \frac{m-1}{2} \alpha \right)^2 \geq 0.$$

In an analogous fashion we obtain

$$\begin{aligned}
 R_{m+1}(t) - 2t + \eta + \eta^{-1} &= \eta^{-1}(T_{m+1}(t) + 1) - 2(T_m(t) + t) + \eta(T_{m-1}(t) + 1) \\
 &= 2\eta^{-1} \cos^2 \frac{m+1}{2} \alpha - 4 \cos \frac{m+1}{2} \alpha \cos \frac{m-1}{2} \alpha \\
 &\quad + 2\eta \cos^2 \frac{m-1}{2} \alpha \\
 (3.10) \qquad \qquad \qquad &= 2\eta^{-1} \left(\cos \frac{m+1}{2} \alpha - \eta \cos \frac{m-1}{2} \alpha \right)^2
 \end{aligned}$$

$$(3.11) \qquad \qquad \qquad = -2\delta^{-1} \left(\cos \frac{m+1}{2} \alpha + \delta \cos \frac{m-1}{2} \alpha \right)^2 \leq 0.$$

Combining (3.8) and (3.10) and using $2t - \eta - \eta^{-1} = 2(t + a)$ yields the desired result. \square

3.2. Algorithm for finding best polynomial approximation to $1/x$. We now assume that we are given a matrix A , and bounds for its eigenvalues denoted by λ_{\min} and λ_{\max} . We will use the result from Theorem 3.3 to construct the polynomial $q_m(A)$ which approximates A^{-1} . We first write the recurrence relation for $q_{m+1}(x) = 2\sigma Q_{m+1}(2\sigma x - a)$:

$$Q_{m+1}(2\sigma x - a) = \eta[-2 + 2(2\sigma x - a)Q_m(2\sigma x - a) - \eta Q_{m-1}(2\sigma x - a)].$$

Multiplying by 2σ then gives

$$q_{m+1}(x) = \eta[-4\sigma + 2\sigma(2\sigma x - a)Q_m(2\sigma x - a) - 2\sigma\eta Q_{m-1}(2\sigma x - a)].$$

We then have the following algorithm in which the formulae are obtained by writing η , σ and a in terms of λ_{\max} and λ_{\min} . The polynomials $q_m(x)$ are written in terms of two parameters, χ and δ , where δ is defined in (3.2) and for χ we have

$$(3.12) \qquad \qquad \qquad \chi = \frac{4}{(\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}})^2},$$

Algorithm 3.5. Set $\mu_0 = 1/\lambda_{\max}$ and $\mu_1 = 1/\lambda_{\min}$.

1. Calculate the 0-th order polynomial q_0 and the first order polynomial q_1 :

$$q_0(x) = \frac{1}{2}(\mu_0 + \mu_1), \quad \text{and} \quad q_1(x) = \frac{1}{2}(\sqrt{\mu_0} + \sqrt{\mu_1})^2 - \mu_0\mu_1 x.$$

2. For $k = 1, \dots, m-1$, q_{k+1} written as a correction to q_k is computed as follows:

$$\begin{aligned}
 s_{k+1}(x) &= \frac{4\mu_0\mu_1}{(\sqrt{\mu_0} + \sqrt{\mu_1})^2} [1 - q_k(x)x] + \delta^2 [q_k(x) - q_{k-1}(x)] \\
 &= \frac{4\mu_0\mu_1}{(\sqrt{\mu_0} + \sqrt{\mu_1})^2} [1 - q_k(x)x] + \delta^2 s_k(x) \\
 q_{k+1}(x) &= q_k(x) + s_{k+1}(x).
 \end{aligned}$$

The reason to write q_{k+1} as a correction to q_k is to show that such iterations look like iterations in a defect-correction method: First computing the residual $[1 - q_k(x)x]$, and then trying to correct it by adding an additional term. One can also easily see that for any initial q_0 and q_1 , if the sequence $q_k(x)$ converges, then it converges to x^{-1} . In another word, choosing q_0 and q_1 different from what they are above, will not generate the sequence of best approximations to x^{-1} , but still this sequence will converge to x^{-1} .

In the remaining sections we will show how the best polynomial approximation to $1/x$ can be utilized in multilevel methods, which results in efficient and often optimal order solution algorithms for symmetric positive definite systems of finite element equations, as they arise for instance from discretization of elliptic partial differential equations.

4. APPLICATION TO MULTILEVEL METHODS

Example 1. A classical choice of $q^{(k)}$ is (2.26) where $p^{(k)}$ is a properly scaled and shifted Chebyshev polynomial satisfying the condition $p^{(k)}(x) \leq 0 \quad \forall t \in [\rho_1^{-1}, \rho_0^{-1}]$. For degree two this polynomial is given by

$$(4.1) \quad p^{(k)}(x) = p(x) = \rho_0 \rho_1 \left(\frac{1}{\rho_0} - x \right) \left(\frac{1}{\rho_1} - x \right)$$

which results in

$$q^{(k)}(x) = q(x) = \rho_0 + \rho_1 - \rho_0 \rho_1 x.$$

For this choice,

$$\begin{aligned} r_0 &= \min_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q(x) = [x q(x)] \Big|_{x=\frac{1}{\rho_1}} = 1, \\ r_1 &= \max_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q(x) = [x q(x)] \Big|_{x=\frac{\rho_0+\rho_1}{2\rho_0\rho_1}} = \frac{(\rho_0 + \rho_1)^2}{4\rho_0\rho_1}. \end{aligned}$$

Hence the uniform bound (2.48) reads

$$\frac{\theta_1}{\theta_0} \frac{(\rho_0 + \rho_1)^2}{4\rho_0\rho_1} \leq \frac{\rho_1}{\rho_0}$$

which requires a uniform approximation property such that

$$\frac{\theta_1}{\theta_0} \leq \frac{4\rho_1^2}{(\rho_0 + \rho_1)^2} = \frac{4\bar{\kappa}^2}{(1 + \bar{\kappa})^2},$$

where we denoted by $\bar{\kappa} = \frac{\rho_1}{\rho_0}$.

Example 2. This example is analysis of AMLI method with the polynomial derived in Theorem 3.3. Let Q_m is the best approximation from \mathcal{P}_m to $\frac{1}{t+a}$ in the L_∞ norm on $[-1, 1]$. We then set

$$q_m(x) = 2\sigma Q_m(2\sigma x - a)$$

where $x = (t+a)/(2\sigma)$. Recall again that from (3.2), we have $\eta < 0$, and $|\eta| = \delta$.

$$(4.2) \quad \begin{aligned} x q_m(x) &= 2\sigma x Q_m(2\sigma x - a) = (t+a) Q_m(t) \\ &= 1 - \frac{2\eta^m}{(\eta - \eta^{-1})^2} R_{m+1}(t) = 1 - \frac{2(-1)^m \delta^m}{(\delta - \delta^{-1})^2} R_{m+1}(t), \quad t \in [-1, 1]. \end{aligned}$$

Combining (3.7) with (4.2) we obtain the estimate

$$(4.3) \quad \frac{\max_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q_m(x)}{\min_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q_m(x)} \leq \frac{\max_{t \in [-1, 1]} \left(1 + \frac{4\delta^m}{(\delta - \delta^{-1})^2} (t + a) \right)}{\min_{t \in [-1, 1]} \left(1 - \frac{4\delta^m}{(\delta - \delta^{-1})^2} (t + a) \right)} \leq \frac{1 + \frac{4\delta^m}{(\delta - \delta^{-1})^2} (1 + a)}{1 - \frac{4\delta^m}{(\delta - \delta^{-1})^2} (1 + a)}.$$

Substituting $\delta = (\sqrt{\kappa} - 1) / (\sqrt{\kappa} + 1)$ and $(1 + a) = (2\kappa) / (\kappa - 1)$ in the right hand side of (4.3) we get an estimate that depends on the condition number κ

$$(4.4) \quad \frac{\max_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q_m(x)}{\min_{x \in [\rho_1^{-1}, \rho_0^{-1}]} x q_m(x)} \leq \frac{2 + \delta^m(\kappa - 1)}{2 - \delta^m(\kappa - 1)}$$

If the degree m of the polynomial is chosen large enough, that is, if

$$\frac{2 + \bar{\delta}^m(\bar{\kappa} - 1)}{2 - \bar{\delta}^m(\bar{\kappa} - 1)} \leq \bar{\kappa} \frac{\theta_0}{\theta_1} =: \bar{\kappa},$$

for some number $\bar{\kappa} \geq 1$, where $\bar{\delta} = \frac{\sqrt{\bar{\kappa}} - 1}{\sqrt{\bar{\kappa}} + 1}$, or, equivalently,

$$m \geq \frac{\log \frac{2(\bar{\kappa}-1)}{(\bar{\kappa}-1)(\bar{\kappa}+1)}}{\log \bar{\delta}}$$

for given constants θ_0 and θ_1 in (2.35) then $\bar{\kappa}$ is a uniform bound for the condition number $\kappa = \kappa(B^{(\ell)^{-1}}A^{(\ell)})$, i.e., $\kappa \leq \bar{\kappa}$ holds for any number of levels ℓ .

The best linear approximation to $\frac{1}{x}$ on $[\rho_1^{-1}, \rho_0^{-1}]$ is given by

$$q(x) = \frac{1}{2}(\sqrt{\rho_0} + \sqrt{\rho_1})^2 - \rho_0\rho_1x.$$

In this case the estimate (4.4) shows that a uniform condition number bound $\bar{\kappa} = \frac{\rho_1}{\rho_0}$ requires a uniform approximation property (2.35) with θ_0 and θ_1 satisfying

$$\frac{\theta_1}{\theta_0} \leq \frac{\bar{\kappa}(1 + 2\sqrt{\bar{\kappa}} - \bar{\kappa})}{3 - 2\sqrt{\bar{\kappa}} + \bar{\kappa}}.$$

For comparison, if we would like to have $\bar{\kappa} \leq 3$ according to (4.4) we need $\frac{\theta_1}{\theta_0} \leq \sqrt{3}$, whereas the Chebyshev polynomial in Example 1 yields the same upper bound on the condition number already for $\frac{\theta_1}{\theta_0} \leq \frac{5}{4}$.

Example 3. One interesting application of the best polynomial approximation to $\frac{1}{x}$ is in constructing a smoother for any AMG (or AMLI) method. In order to use $q_m(A)$ as smoother for A , we have to make sure that $q_m(x) > 0$ for all x in $(0, \bar{\lambda}]$ where $\bar{\lambda}$ is an upper bound on the spectrum of A . In practice, when estimates on $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ are not available one can use

$$(4.5) \quad \bar{\lambda} = \|A\|_{\ell^\infty}$$

and construct the best approximation $q_m(x)$ to $\frac{1}{x}$ on the interval $[\frac{\bar{\lambda}}{\mu}, \bar{\lambda}]$ where $\mu > 1$ is a constant. Note that $q_m(x) > 0$ for all x in $(0, \bar{\lambda}]$ if $q_m(x)x > 0$ for all $x \in [\frac{\bar{\lambda}}{\mu}, \bar{\lambda}]$. The latter condition holds true if

$$(4.6) \quad 1 - \frac{2(-1)^m \delta^m}{(\delta - \delta^{-1})^2} R_{m+1}(t) > 0.$$

We first estimate below the left side of this inequality as follows

$$\begin{aligned} 1 - \frac{2(-1)^m \delta^m}{(\delta - \delta^{-1})^2} R_{m+1}(t) &\geq 1 - \frac{2\delta^m}{(\delta - \delta^{-1})^2} |R_{m+1}(t)| \\ &\geq 1 - \frac{2\delta^m}{(\delta - \delta^{-1})^2} (2t + \delta + \delta^{-1}) \\ &= 1 - \frac{4\delta^m}{(\delta - \delta^{-1})^2} (t + a) \\ &\geq 1 - \frac{4\delta^m}{(\delta - \delta^{-1})^2} (1 + a) = 1 - \frac{(a - \sqrt{a^2 - 1})^m}{a - 1}, \end{aligned}$$

where we have used that $\delta = a - \sqrt{a^2 - 1}$ and $(\delta - \delta^{-1})^2 = 4(a^2 - 1)$. As a consequence, a sufficient condition for the inequality (4.6) to hold then is given by

$$(4.7) \quad \left(\frac{\sqrt{\mu} - 1}{\sqrt{\mu} + 1} \right)^m < \frac{2}{\mu - 1}.$$

An upper bound on the damping factor of the smoother on the error components that correspond to eigenvalues in the interval $[\frac{\bar{\lambda}}{\mu}, \bar{\lambda}]$ is as follows

$$(4.8) \quad \rho(I - q_m(A)A) \leq \frac{\mu - 1}{2} \left(\frac{\sqrt{\mu} - 1}{\sqrt{\mu} + 1} \right)^m.$$

For example, if $\mu = 4$ the condition (4.7) holds for all $m \geq 1$. Choosing $m = 2$ in this case results in a damping factor of *at most* $\frac{1}{6}$ for all error components in the span of eigenvectors whose eigenvalues are in the interval $[\frac{\bar{\lambda}}{4}, \bar{\lambda}]$.

If $\mu = 8$ the condition (4.7) for positivity of $q_m(x)$ is satisfied for all $m \geq 2$. Choosing $m = 3$ in this case the estimate of the damping factor (right hand side of (4.8)) is given by $\frac{7}{2} \left(\frac{\sqrt{8} - 1}{\sqrt{8} + 1} \right)^3 \approx 0.381276$ for the interval $[\frac{\bar{\lambda}}{8}, \bar{\lambda}]$. To calculate the damping factor in other cases is also rather straightforward.

5. CORRESPONDENCE AND DIFFERENCES BETWEEN THE STANDARD AMLI METHODS AND AMG

Finally, we would like to comment on the correspondence and differences between the ‘‘smoother’’ \bar{M} and the prolongation used in AMG and the ones used in the standard AMLI

method. The standard AMLI method, as introduced in [7, 8] uses f-smoothing only, i.e.,

$$(5.1) \quad \bar{M}^{-1} = \begin{bmatrix} 2C_{11}^{-1} - C_{11}^{-1}A_{11}C_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix}.$$

One possible implementation (that corresponds to the multiplicative variant) yields the preconditioner

$$(5.2) \quad \begin{aligned} \tilde{B}^{-1} &= \begin{bmatrix} C_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} -C_{11}^{-1}A_{12} \\ I \end{bmatrix} Z^{-1} [-A_{21}C_{11}^{-1}, I] \\ &= \begin{bmatrix} C_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \\ &+ \begin{bmatrix} I - C_{11}^{-1}A_{11} & -C_{11}^{-1}A_{12} \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 \\ I \end{bmatrix} Z^{-1} [0, I] \begin{bmatrix} I - A_{11}C_{11}^{-1} & 0 \\ -A_{21}C_{11}^{-1} & I \end{bmatrix} \\ &= M^{-1} + (I - M^{-T}A) P Z^{-1} P^T (I - AM^{-1}), \end{aligned}$$

which uses the symmetrized smoother (5.1). Then, in order to write B^{-1} in the form (2.3) one has to choose

$$(5.3) \quad P = \begin{bmatrix} 0 \\ I \end{bmatrix}.$$

We notice that the simple form of (5.3) is related to the fact that the AMLI preconditioner is defined for the hierarchical two-level matrix $\tilde{A} = J^T A J$, which contains already the coarse-level matrix as a sub-matrix in its lower right block, i.e.,

$$A_H = [0, I] \tilde{A} \begin{bmatrix} 0 \\ I \end{bmatrix}.$$

This, however, is in accordance with the Galerkin relation $A_H = P^T A P$ as is used in AMG methods.

We conclude that the polynomial acceleration techniques that we studied here can be exploited in various ways in the implementation of AMLI and/or AMG based preconditioners, since both can be viewed as inexact two-level methods as we described in Section 2.1. The performance of both type of methods crucially depends on the particular choice of the polynomial $q_{\nu-1}(\cdot)$ in equation (2.15).

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APPENDIX A. PROOF OF THEOREM 3.3

With the intent to keep this article self-contained, in this section we give another proof of Theorem 3.3, without using symbolic computation techniques. We start by defining several trigonometric functions which are used in the proof of the theorem.

$$(A.1) \quad c_o(\alpha) = \cos \ell\alpha + d \cos(\ell - 1)\alpha,$$

$$(A.2) \quad s_o(\alpha) = \sin \ell\alpha + d \sin(\ell - 1)\alpha,$$

$$(A.3) \quad s_e(\alpha) = \sin \frac{(2\ell + 1)\alpha}{2} + d \sin \frac{(2\ell - 1)\alpha}{2},$$

$$(A.4) \quad c_e(\alpha) = \cos \frac{(2\ell + 1)\alpha}{2} + d \cos \frac{(2\ell - 1)\alpha}{2}.$$

We first show that $Q_m(t)$ as defined in the statement of Theorem 3.3 is indeed a polynomial of degree at most m .

Lemma A.1. *Let $m \geq 1$ be a fixed integer and*

$$Q(t) = \frac{1}{t+a} \left(1 - \frac{2\eta^m}{(\eta - \eta^{-1})^2} R_{m+1}(t) \right),$$

where

$$R_{m+1}(t) = \eta^{-1}T_{m+1}(t) - 2T_m(t) + \eta T_{m-1}(t).$$

Then $Q(t) \in \mathcal{P}_m(t)$.

Proof. We consider

$$r(t) = 1 - \frac{2(\eta)^m}{(\eta - \eta^{-1})^2} R_{m+1}(t)$$

which is obviously a polynomial in t of degree less than or equal to $(m+1)$. Since $Q(t) = r(t)/(t+a)$, it is enough to show that $r(-a) = 0$ and hence, $r(t)$ is divisible by $(t+a)$. We first compute $R_{m+1}(-a)$, noting that

$$T_k(-a) = \frac{1}{2}(\eta^k + \eta^{-k}).$$

Therefore,

$$\begin{aligned} R_{m+1}(-a) &= \frac{1}{2}(\eta^m + \eta^{-m-2} - 2\eta^m - 2\eta^{-m} + \eta^m + \eta^{2-m}) \\ &= \frac{1}{2}(\eta^{-m-2} - 2\eta^{-m} + \eta^{2-m}) \end{aligned}$$

For $r(-a)$ we then have

$$\begin{aligned} r(-a) &= 1 - \frac{1}{(\eta - \eta^{-1})^2} \eta^m (\eta^{-m-2} - 2\eta^{-m} + \eta^{2-m}) \\ &= 1 - \frac{\eta^{-2} - 2 + \eta^2}{(\eta - \eta^{-1})^2} = 0. \end{aligned}$$

□

We now give the proof of Theorem 3.3. The proof uses two auxiliary results, on the interlacing of zeroes of the trigonometric functions defined by (A.1)-(A.4), namely Lemma A.4, and Lemma A.5. We stated and proved these results in subsection A.1.

Proof of Theorem 3.3. From Lemma A.1, we know that Q_m is a polynomial. To show that $Q_m(t)$ is the polynomial of best approximation, we need to show that the error $e(t) = \left(\frac{1}{t+a} - Q_m(t)\right)$ has $(m+2)$ points of Chebyshev alternance, that is, to show that there exist points $t_1 < t_2 \dots < t_{m+2}$, such that

$$|e(t_1)| = \left| \frac{1}{t+a} - Q_m(t) \right|_{\infty}, \quad \text{and} \quad e(t_k) = -e(t_{k-1}), k = 2, 3, \dots, (m+2).$$

Clearly,

$$e(t) = (-1)^m \frac{4\delta^m}{(\delta - \delta^{-1})^2} \frac{R_{m+1}(t)}{2t + \delta + \delta^{-1}}.$$

We put $t = \cos \alpha$, for $\alpha \in [0, \pi]$, take $d = \delta < 1$ in definitions (A.1)-(A.4) and apply the identities from the proof of Lemma 3.4. We then find that if m is odd, $m = (2\ell - 1)$, then

$$\begin{aligned} R_{m+1}(t) &= -(2t + \delta + \delta^{-1}) + 2\delta^{-1} s_o^2(\alpha) \geq -(2t + \delta + \delta^{-1}) \\ R_{m+1}(t) &= 2t + \delta + \delta^{-1} - 2\delta^{-1} c_o^2(\alpha) \leq 2t + \delta + \delta^{-1} \end{aligned}$$

If m is even, $m = 2\ell$, in an analogous fashion we have

$$\begin{aligned} R_{m+1}(t) &= -(2t + \delta + \delta^{-1}) + 2\delta^{-1} s_e^2(\alpha) \geq -(2t + \delta + \delta^{-1}) \\ R_{m+1}(t) &= 2t + \delta + \delta^{-1} - 2\delta^{-1} c_e^2(\alpha) \leq 2t + \delta + \delta^{-1} \end{aligned}$$

From these relations it is easy to see that in both cases m odd or even,

$$(A.5) \quad -(2t + \delta + \delta^{-1}) \leq R_{m+1}(t) \leq 2t + \delta + \delta^{-1},$$

and hence $|R_{m+1}(t)| \leq 2t + \delta + \delta^{-1}$ (this is the same as in Lemma 3.4, but written in terms of δ). Clearly, we have equalities in (A.5) when $t = \arccos(\alpha)$, and α is a zero of c_o and s_o in case $m = (2\ell - 1)$, and a zero of c_e and s_e in case $m = 2\ell$. Thus, since the zeros of these functions interlace (see Lemma A.4, and Lemma A.5 below) we may conclude that there exist $\{t_k\}_{k=1}^{m+2}$, such that

$$(A.6) \quad R_{m+1}(t_k) = \pm(-1)^k(2t_k + \delta + \delta^{-1}).$$

Indeed, it is easy to check that Lemma A.4 (item 3.), and Lemma A.5 (item 3.), imply that when $m = (2\ell - 1)$, the $(2\ell + 1)$ points of Chebyshev alternance for $e(t)$ are given in Lemma A.4 and are $\{\cos \alpha_k\}_{k=0}^{2\ell}$, and analogously, for $m = 2\ell$, the points of Chebyshev alternance of $e(t)$ are given in Lemma A.5 and they are $\{\cos \beta_k\}_{k=0}^{2\ell+1}$. Finally, by the Chebyshev alternating theorem we conclude that $Q_m(t)$ is the best polynomial approximation to $\frac{1}{t+a}$ in the uniform norm, and for the error we have

$$E_{[-1,1]} = \frac{4\delta^m}{(\delta - \delta^{-1})^2}.$$

This completes the proof of the theorem. \square

A.1. Auxiliary results. This subsection contains two auxiliary results Lemma A.4, and Lemma A.5, used in the proof of Theorem 3.3. The proof of these two lemmas requires series of inequalities, most of which are well known. We state and prove these here for completeness. Here is a Lemma, which gives known trigonometric identities and can be found in many texts (see e.g. [44]).

Lemma A.2. *The following identity holds*

$$(A.7) \quad \sin \frac{\alpha}{2} \left[1 + 2 \sum_{k=1}^{\ell} \cos k\alpha \right] = \sin \frac{(2\ell + 1)\alpha}{2}.$$

Proof. Set $a_j = \sin \frac{(2j+1)\alpha}{2}$, $j = 0, \dots, \ell$ and recall that, for $j = 1, 2, \dots, \ell$ we have

$$2 \cos j\alpha \sin \frac{\alpha}{2} = \sin \frac{(2j+1)\alpha}{2} - \sin \frac{(2j-1)\alpha}{2} = a_j - a_{j-1}.$$

Therefore,

$$\begin{aligned} \sin \frac{\alpha}{2} \left(1 + 2 \sum_{j=1}^{\ell} \cos j\alpha \right) &= \sin \frac{\alpha}{2} + \sum_{j=1}^{\ell} 2 \sin \frac{\alpha}{2} \cos j\alpha \\ &= a_0 + \sum_{j=1}^{\ell} (a_j - a_{j-1}) = a_{\ell}, \end{aligned}$$

which completes the proof. \square

Next, we show an upper bound on the number of zeros of c_o and s_e for fixed ℓ .

Lemma A.3. *Let $\ell \geq 1$ be a fixed integer, $0 < d < 1$ and $c_o(\alpha)$ and $s_e(\alpha)$ be defined as in (A.1) and (A.3) respectively. Then c_o has at most ℓ zeros in the interval $[0, \pi]$ and s_e has at most $(\ell + 1)$ zeros in the interval $[0, \pi]$.*

Proof. We first prove that $c_o(\alpha)$ has no more than ℓ zeros in $[0, \pi]$. Set $t = \cos \alpha$, and then

$$c_o(\arccos(t)) = T_\ell(t) + dT_{\ell-1}(t),$$

and hence $c_o(\arccos(t))$ is a polynomial of degree ℓ in t . If we assume that $c_o(\alpha)$ has more than ℓ zeros for $\alpha \in [0, \pi]$, then the polynomial $c_o(\arccos(t))$ would have more than ℓ zeros, which would imply $c_o(\alpha) \equiv 0$, and this obviously is a contradiction.

We now prove that $s_e(\alpha)$ has at most $(\ell + 1)$ zeros. From Lemma A.2, we have that

$$\begin{aligned} s_e(\alpha) &= \sin \frac{(2\ell + 1)\alpha}{2} + d \sin \frac{(2\ell - 1)\alpha}{2} \\ &= \sin \frac{\alpha}{2} \left[1 + 2 \sum_{k=1}^{\ell} \cos k\alpha \right] + d \sin \frac{\alpha}{2} \left[1 + 2 \sum_{k=1}^{\ell-1} \cos k\alpha \right] \\ &= \sin \frac{\alpha}{2} \left[(1 + d) + 2 \cos \ell\alpha + (2 + 2d) \sum_{k=1}^{\ell-1} \cos k\alpha \right]. \end{aligned}$$

Hence we have for $\alpha = \arccos(t)$, $t \in [-1, 1]$

$$s_e(\arccos(t)) = \sin \frac{\arccos(t)}{2} q(t),$$

where $q(t)$ is a polynomial of degree ℓ ,

$$q(t) = \left[(1 + d) + 2T_\ell(t) + (2 + 2d) \sum_{k=1}^{\ell-1} T_k(t) \right].$$

Clearly, $q(t)$ has at most ℓ zeros. Another zero of $s_e(\arccos(t))$ is at $t = 1$ (or $\alpha = 0$). Hence there are at most $(\ell + 1)$ zeros of s_e in the interval $[0, \pi]$. \square

The following two lemmas give more precise estimates on the location of the zeros of $c_o(\alpha)$ and $s_o(\alpha)$ ($s_e(\alpha)$ and $c_e(\alpha)$, respectively).

Lemma A.4. *Let $\ell \geq 1$ be a given integer, and $0 < d < 1$. Then,*

1. *The function $c_o(\alpha)$ has exactly ℓ zeros $\alpha_{2k-1} \in \left(\frac{(2k-1)\pi}{2\ell}, \frac{k\pi}{\ell} \right)$, $k = 1, 2, \dots, \ell$ in the open interval $(0, \pi)$.*
2. *The function $s_o(\alpha)$ has exactly $(\ell + 1)$ zeros in the interval $[0, \pi]$: $\alpha_0 = 0$, $\alpha_{2\ell} = \pi$ and $(\ell - 1)$ zeros $\alpha_{2k} \in \left(\frac{k\pi}{\ell}, \frac{(2k+1)\pi}{2\ell} \right)$, $k = 1, 2, \dots, (\ell - 1)$.*
3. *The zeros of $c_o(\alpha)$ and $s_o(\alpha)$ interlace, namely*

$$0 = \alpha_0 < \alpha_1 < \alpha_2 < \dots < \alpha_{2\ell-2} < \alpha_{2\ell-1} < \alpha_{2\ell} = \pi.$$

The total number of zeros (either zeros of c_o or zeros of s_o) is $(2\ell + 1)$.

Proof. We calculate the value of $c_o(\alpha)$ at the end points of each interval $\left(\frac{(2k-1)\pi}{2\ell}, \frac{k\pi}{\ell}\right)$. For $k = 1, \dots, \ell$, we have

$$\begin{aligned} c_o\left(\frac{(2k-1)\pi}{2\ell}\right) &= \cos\frac{(2k-1)\pi}{2} + d\cos\frac{(\ell-1)(2k-1)\pi}{2\ell} \\ &= d\cos\left(\frac{(2k-1)\pi}{2} - \frac{(2k-1)\pi}{2\ell}\right) \\ &= d\sin\frac{(2k-1)\pi}{2}\sin\frac{(2k-1)\pi}{2\ell} = (-1)^{k-1}d\sin\frac{(2k-1)\pi}{2\ell} \\ c_o\left(\frac{k\pi}{\ell}\right) &= \cos(k\pi) + d\cos\left(k\pi - \frac{k\pi}{\ell}\right) \\ &= (-1)^k + d\cos(k\pi)\cos\frac{k\pi}{\ell} = (-1)^k\left[1 + d\cos\frac{k\pi}{\ell}\right]. \end{aligned}$$

Since for $0 < d < 1$ and $k = 1, 2, \dots, \ell$, we have that

$$d\sin\frac{(2k-1)\pi}{2\ell} > 0, \quad \text{and} \quad \left[1 + d\cos\frac{k\pi}{\ell}\right] > 0,$$

we may conclude that

$$(A.8) \quad \text{sign } c_o\left(\frac{(2k-1)\pi}{2\ell}\right) = (-1)^{k-1}, \quad \text{sign } c_o\left(\frac{k\pi}{\ell}\right) = (-1)^k.$$

Hence, $c_o(\alpha)$ has at least one zero in each of the open intervals $\left(\frac{(2k-1)\pi}{2\ell}, \frac{k\pi}{\ell}\right)$. These are ℓ disjoint intervals and thus $c_o(\alpha)$ has at least ℓ different zeros. Since from Lemma A.3 we know that $c_o(\alpha)$ has at most ℓ zeros, we conclude that $c_o(\alpha)$ has exactly ℓ zeros in $[0, \pi]$, and we denote these with α_{2k-1} . This completes the proof of the first item.

We note here that the number of zeros of c_o and the intervals in which the zeros of c_o are located is independent of the particular value of d , as long as $0 < d < 1$.

We move on, to prove item 2. in the statement of the lemma. We take the derivative of s_o with respect to α , to obtain that

$$\frac{ds_o}{d\alpha} = \ell\left[\cos\ell\alpha + \frac{\ell-1}{\ell}d\cos(\ell-1)\alpha\right].$$

According to what we proved above for $c_o(\alpha)$, (but with d replaced by $\frac{\ell-1}{\ell}d$), the derivative $\frac{ds}{d\alpha}$ has exactly ℓ different zeros, and therefore $s_o(\alpha)$ cannot have more than $(\ell+1)$ different zeros in $[0, \pi]$.

It is immediate to verify that $s(0) = s(\pi) = 0$. We will show now that $s_o(\alpha)$ changes sign in each of the open intervals $\left(\frac{k\pi}{\ell}, \frac{(2k+1)\pi}{2\ell}\right)$, $k = 1, 2, \dots, (\ell-1)$, and hence has at least one zero in every such interval. Together with the end points this will give all the zeros of

$s_o(\alpha)$. Calculating $s_o\left(\frac{k\pi}{\ell}\right)$ and $s_o\left(\frac{(2k+1)\pi}{2\ell}\right)$ $k = 1, 2, \dots, (\ell - 1)$ gives

$$\begin{aligned} s_o\left(\frac{k\pi}{\ell}\right) &= \sin(k\pi) + d \sin\left(k\pi - \frac{k\pi}{\ell}\right) \\ &= -d \cos(k\pi) \sin \frac{k\pi}{\ell} = (-1)^{k+1} d \sin \frac{k\pi}{\ell}. \\ s_o\left(\frac{(2k+1)\pi}{2\ell}\right) &= \sin \frac{(2k+1)\pi}{2} + d \sin \frac{(\ell-1)(2k+1)\pi}{2\ell} \\ &= (-1)^k + d \sin\left(\frac{(2k+1)\pi}{2} - \frac{(2k+1)\pi}{2\ell}\right) \\ &= (-1)^k + d(-1)^k \cos \frac{(2k+1)\pi}{2\ell} = (-1)^k \left[1 + d \cos \frac{(2k+1)\pi}{2\ell}\right]. \end{aligned}$$

Clearly, for $k = 1, \dots, \ell - 1$ and $0 < d < 1$ we have that $d \sin \frac{k\pi}{\ell} > 0$ and that $\left[1 + d \cos \frac{(2k+1)\pi}{2\ell}\right] > 0$, which leads to

$$(A.9) \quad \text{sign } s_o\left(\frac{k\pi}{\ell}\right) = (-1)^{k+1}, \quad \text{sign } s_o\left(\frac{(2k+1)\pi}{2\ell}\right) = (-1)^k,$$

and (A.9) implies that in addition to the end points $\alpha_0 = 0$ and $\alpha_{2\ell} = \pi$, we have exactly one zeros α_{2k} in each of the intervals $\left(\frac{k\pi}{\ell}, \frac{(2k+1)\pi}{2\ell}\right)$.

To show that item 3. holds is easy, because for $k = 1, \dots, (\ell - 1)$ we have that α_{2k-1} is to the left of $\frac{k\pi}{\ell}$, while α_{2k} is to the right of $\frac{k\pi}{\ell}$. Therefore,

$$\alpha_{2k-1} < \frac{k\pi}{\ell} < \alpha_{2k} < \frac{(2k+1)\pi}{2\ell} < \alpha_{2k+1} < \frac{(k+1)\pi}{\ell}.$$

Since for all $j = 1, \dots, 2\ell$, $0 = \alpha_0 < \alpha_j$ and for $j = 0, \dots, (2\ell - 1)$, $\alpha_j < \alpha_{2\ell} = \pi$, the proof of item 3. is concluded. \square

Similar lemma and with similar proof (which we only sketch below) holds for ℓ replaced by $(\ell + \frac{1}{2})$.

Lemma A.5. *Let $\ell \geq 1$ be a given integer, $0 < d < 1$. Then,*

1. *The function $s_e(\alpha)$ has exactly $(\ell + 1)$ zeros: $\beta_0 = 0$, and $\beta_{2k} \in \left(\frac{2k\pi}{2\ell+1}, \frac{(2k+1)\pi}{2\ell+1}\right)$, $k = 1, \dots, \ell$.*
2. *The function $c_e(\alpha)$ has exactly $(\ell + 1)$ zeros: $\beta_{2k-1} \in \left(\frac{(2k-1)\pi}{2\ell+1}, \frac{2k\pi}{2\ell+1}\right)$, $k = 1, \dots, \ell$, and $\beta_{2\ell+1} = \pi$.*
3. *The zeros of $s_e(\alpha)$ and $c_e(\alpha)$ interlace, namely*

$$0 = \beta_0 < \beta_1 < \beta_2 < \dots < \beta_{2\ell-1} < \beta_{2\ell} < \beta_{2\ell+1} = \pi.$$

The total number of zeros (either zeros of s_e or zeros of c_e) is $(2\ell + 2)$.

Proof. To prove the statement for s_e we proceed as in Lemma A.4. Since the intervals $\left(\frac{2k\pi}{2\ell+1}, \frac{(2k+1)\pi}{2\ell+1}\right)$ are disjoint, and s_e has ℓ zeros in $(0, \pi]$, we only need to show that $s_e(\alpha)$ changes sign in each interval. For $k = 1, \dots, \ell$ we calculate

$$\begin{aligned}
s_e\left(\frac{2k\pi}{2\ell+1}\right) &= \sin k\pi + d \sin \frac{(2\ell-1)(k\pi)}{2\ell+1} \\
&= d \sin\left(k\pi - \frac{2k\pi}{2\ell+1}\right) \\
&= -d \cos k\pi \sin \frac{2k\pi}{2\ell+1} = (-1)^{k+1} d \sin \frac{2k\pi}{2\ell+1} \\
s_e\left(\frac{(2k+1)\pi}{2\ell+1}\right) &= \sin \frac{(2k+1)\pi}{2} + d \sin \frac{(2\ell-1)(2k+1)\pi}{2(2\ell+1)} \\
&= (-1)^k + d \sin\left(\frac{(2k+1)\pi}{2} - \frac{(2k+1)\pi}{2\ell+1}\right) \\
&= (-1)^k + d \sin \frac{(2k+1)\pi}{2} \cos \frac{(2k+1)\pi}{2\ell+1} = (-1)^k \left[1 + d \cos \frac{(2k+1)\pi}{2\ell+1}\right].
\end{aligned}$$

Since $0 < d < 1$ we conclude that $s_e(\alpha)$ changes sign in every interval. Obviously also $s_e(0) = 0$, and hence $s_e(\alpha)$ has exactly $(\ell + 1)$ zeros in the interval $[0, \pi]$.

Next, to prove the statement for the zeros of $c_e(\alpha)$, we argue analogously as in proving the second part of Lemma A.4 to show that c_e cannot have more than $(\ell + 1)$ zeros in $[0, \pi]$. To check that c_e changes sign in each of the intervals $\left(\frac{(2k-1)\pi}{2\ell+1}, \frac{2k\pi}{2\ell+1}\right)$, is straightforward, and analogous to what we did for $s_e(\alpha)$. That the ordering of the zeros of $c_e(\alpha)$ and $s_e(\alpha)$ stated in item 3. holds is also verified in a fashion similar to the proof of item 3. of Lemma A.4. \square