

On the decay of the off-diagonal singular values in cyclic reduction*

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Abstract

It was recently observed in [9] that the singular values of the off-diagonal blocks of the matrix sequences generated by the Cyclic Reduction algorithm decay exponentially. This property was used to solve, with a higher efficiency, certain quadratic matrix equations encountered in the analysis of queuing models. In this paper, we provide a sharp theoretical bound to the basis of this exponential decay together with a tool for its estimation based on a rational interpolation problem. Applications to solving $n \times n$ block tridiagonal block Toeplitz systems with $n \times n$ semiseparable blocks and certain generalized Sylvester equations in $O(n^2 \log n)$ arithmetic operations are shown.

Keywords: Cyclic reduction, quasiseparable matrices, rational interpolation, Sylvester equations, exponential decay, block tridiagonal systems.

AMS subject classifications: 41A20, 60J22, 65F05.

1 Introduction

Cyclic reduction, CR for short, is an algorithm originally introduced by G. H. Golub and R. W. Hockney in [17] for the solution of certain block tridiagonal linear systems coming from the finite difference discretization of elliptic PDEs. It has been later generalized and extended to other contexts, like for instance to the solution of polynomial matrix equations, and has been proven to be a successful method for solving a large class of queuing problems and infinite Markov Chains. We refer the reader to the books [8], [7] and to the survey paper [10] for more details and for the many references to the literature.

Given three $m \times m$ matrices A_{-1} , A_0 , A_1 , and a positive integer n consider the block tridiagonal block Toeplitz matrix $\mathcal{A}_n = \text{trid}_n(A_{-1}, A_0, A_1)$ having block-size n where A_0 is on the main diagonal while A_{-1} is in the lower diagonal and A_1 in the upper diagonal. For a vector $b \in \mathbb{R}^{mn}$, consider the system $\mathcal{A}_n x = b$. Roughly speaking, CR generates three sequences of $m \times m$ matrices $A_{-1}^{(h)}$, $A_0^{(h)}$ and $A_1^{(h)}$, for $h = 0, 1, \dots$, with $A_i^{(0)} = A_i$, $i = -1, 0, 1$, and a sequence of systems $\mathcal{A}_{n_h} x^{(h)} = b^{(h)}$, $\mathcal{A}_{n_h} = \text{trid}_{n_h}(A_{-1}^{(h)}, A_0^{(h)}, A_1^{(h)})$, where $n_h = \lfloor n_{h-1}/2 \rfloor$ and $x^{(h)}$ is a subvector of x . This way, solving a block tridiagonal block-Toeplitz system of block size n is reduced to solving a block tridiagonal block Toeplitz system of size $\lfloor n/2 \rfloor$. The computation of $A_i^{(h)}$ given

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$A_i^{(h-1)}$, for $i = -1, 0, 1$, amounts to perform one matrix inversion and few matrix multiplications for the overall cost per step of $O(m^3)$ arithmetic operations (ops).

Under certain assumptions, customarily verified in many applications, the sequence $A_1^{(h)}$ and/or $A_{-1}^{(h)}$ converge doubly exponentially to zero. This makes CR a powerful tool for solving large or even infinite systems, as well as matrix equations of the kind $A_{-1} + A_0X + A_1X^2 = 0$, typically encountered in the analysis of queuing problems [21], where the unknown is the $m \times m$ matrix X and a solution of spectral radius at most 1 is sought.

In short, the three sequences $A_i^{(h)}$, $i = -1, 0, 1$, which are related to the Schur complements of certain principal submatrices of \mathcal{A}_n , are given by the following matrix recurrences where we report also two additional auxiliary sequences, namely $\tilde{A}^{(h)}$ and $\hat{A}^{(h)}$, which have a role in the solution of quadratic matrix equations and of linear systems when n is not of the kind $2^k - 1$:

$$\begin{aligned} A_0^{(h+1)} &= A_0^{(h)} - A_1^{(h)} S^{(h)} A_{-1}^{(h)} - A_{-1}^{(h)} S^{(h)} A_1^{(h)}, & S^{(h)} &= (A_0^{(h)})^{-1} \\ A_1^{(h+1)} &= -A_1^{(h)} S^{(h)} A_1^{(h)}, & A_{-1}^{(h+1)} &= -A_{-1}^{(h)} S^{(h)} A_{-1}^{(h)}, & h &= 0, 1, \dots \\ \hat{A}^{(h+1)} &= \hat{A}^{(h)} - A_1^{(h)} S^{(h)} A_{-1}^{(h)}, & \tilde{A}^{(h+1)} &= \tilde{A}^{(h)} - A_{-1} S^{(h)} A_1^{(h)} \end{aligned} \quad (1)$$

with $A_0^{(0)} = \tilde{A}^{(0)} = \hat{A}^{(0)} = A_0$, $A_1^{(0)} = A_1$, $A_{-1}^{(0)} = A_{-1}$.

Here we assume that all the matrices $A_0^{(h)}$ generated by the recursion are invertible so that CR can be carried out with no breakdown. This assumption is generally satisfied in the applications.

In many cases of great interest, encountered for instance in the analysis of bi-dimensional random walks, queuing models, network analysis [21], [24], [23], [18], [20], and finite differences discretization of elliptic PDEs [13], the blocks A_{-1} , A_0 and A_1 are tridiagonal or, more generally, banded matrices. This has raised great attention to the computational analysis of this case. The additional tridiagonal structure makes it much cheaper to perform the first steps of CR where the computational cost drops from $O(n^3)$ to $O(n)$ ops. However, after a few steps, the sparse structure of the initial blocks is lost and one has to deal with full, apparently unstructured matrices $A_i^{(h)}$, $i = -1, 0, 1$.

Recently, in [9], it has been observed that if A_{-1} , A_0 and A_1 are tridiagonal, then the matrices $A_i^{(h)}$, even if dense, numerically maintain a property of *quasi-separability*. That is, their submatrices contained in the strict upper triangular part or in the strict lower triangular part, called *off-diagonal submatrices*, have a “small” numerical rank. More formally, it has been proved that if $\sigma_{i,h}$ are the singular values of any off-diagonal submatrix of, say, $A_0^{(h)}$, ordered in non-increasing order, then $\sigma_{i,h} \leq \gamma t^{i/2}$ for some small $\gamma > 0$ and for some $0 < t < 1$. The value of t is such that the matrix $z^2 A_1 + z A_0 + A_{-1}$ is invertible for any complex z such that $t < |z| < t^{-1}$.

The analysis of [9] provides a theoretical explanation of an observed computational property which enables one to implement CR with a high computational efficiency by relying on the properties of quasiseparable matrices [27], [28]. In fact, an efficient implementation of CR has been given based on the software library [11] of hierarchical quasiseparable matrices, and the numerical experiments show the high effectiveness of this approach.

However, the results of [9] provide an under estimate of the decay properties of the singular values of the off-diagonal blocks of $A_{-1}^{(h)}$, $A_0^{(h)}$ and $A_1^{(h)}$. In fact, it turns out that, even in the cases where the matrix polynomial $z^2 A_1 + z A_0 + A_{-1}$ is singular at some point just outside a thin annulus $\mathbb{A}_t = \{z \in \mathbb{C} : t \leq |z| \leq t^{-1}\}$ obtained with some t very close to 1, the observed exponential decay of the singular values is still evident with a basis of the exponential much smaller than the given theoretical bound t .

A typical example is given by the discrete Laplacian matrix where $A_0 = \text{trid}(-1, 4, -1)$, $A_{-1} = A_1 = -I$ so that $t = 1 - 1/(n+1) + O(1/(n+1)^2)$. In this case, for moderately large

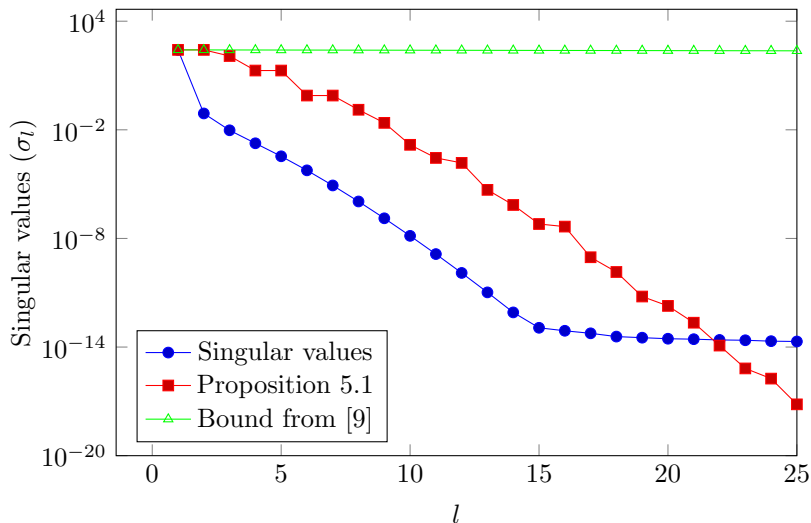


Figure 1: This graph displays the singular values of the largest off-diagonal block of the matrix $H_0 = \lim_h A_0^{(h)}$ computed by means of CR for the Poisson problem where $m = 200$. The red squares denote the upper bound, the blue discs the computed values, the green triangles the bound from [9]. The exponential decay and the sharpness of the bound are evident.

values of n , the bound t^j is still close to 1 for values of j as large as n . As a result, the plot of the upper bounds to the singular values would be an almost horizontal line. On the other hand from the numerical experiments it turns out that the decay of the singular values is still exponential despite the width of the annulus collapses to zero, and the basis of the exponential is much less than t and almost independent of n .

With the tools introduced in this paper, we can capture this property as shown in Figure 1 where the decay of the off-diagonal singular values of the matrix $H_0 = \lim_h A_0^{(h)}$, together with their theoretical upper bounds, are displayed.

In fact, in this paper we provide a different theoretical explanation of the exponential decay of the singular values which relies on an unpublished result of B. Beckermann [3] where the decay of certain singular values associated with some Krylov matrix is expressed in terms of the accuracy of a rational function approximation problem.

This analysis leads to a fast algorithm, which we call *quasiseparable CR* (QCR for short), for solving an $n \times n$ block tridiagonal block Toeplitz system, where the matrix $\text{trid}_n(B, A, C)$ has quasiseparable, say tridiagonal, $m \times m$ blocks A, B, C . The cost of the algorithm is $O(mn \log m + m \log^2 m \log n)$ ops which reduces to $O(n^2 \log n)$ ops for $m = n$. This cost is comparable with that of the fast Poisson solvers [14, Sect. 4.8.4], which apply to the case where $A = \text{trid}_n(-1, 4, 1)$, $B = C = -I$. Unlike the latter algorithms, quasiseparable CR covers a wider and more general class of cases.

We show also an application of QCR to solving a generalized Sylvester equation of the kind

$$\sum_{i=1}^k A_i X B_i = C$$

for given matrices A_i, B_i and C of compatible sizes, in the case where A_i are tridiagonal Toeplitz,

and B_i are quasiseparable matrices. In fact, in this case, the problem is reduced to solve a block tridiagonal block Toeplitz system with quasiseparable blocks. The cost of the solution is again $O(n^2 \log n)$ ops where, for simplicity, we assume that all the matrices involved are $n \times n$.

Decay properties of the off-diagonal blocks of matrix functions have been recently received much attention. In particular, in the paper by M. Benzi and P. Boito and N. Razouk [5] the decay properties of spectral projectors associated with large and sparse Hermitian matrices are investigated. In [19] D. Kressner and A. Susnjara prove a priori bounds for the numerical rank of the off-diagonal blocks of spectral projectors —associated with symmetric banded matrices— by using the best rational approximant of the sign function. In [4] M. Benzi and P. Boito extend previous results on the exponential off-diagonal decay of the entries of analytic functions of banded and sparse matrices to the case where the matrix entries are elements of a C^* -algebra. M. Benzi and V. Simoncini [6] find decay bounds for completely monotonic functions of matrices which are the Kronecker sum of banded or sparse matrices. While C. Canuto, V. Simoncini and M. Verani [12] analyze the decay pattern of the inverses of banded matrices of the form $I \otimes M + M \otimes I$ where M is tridiagonal, symmetric and positive definite. In [13], S. Chandrasekaran, P. Dewilde, M. Gu, and N. Somasunderam analyze the numerical rank of the off-diagonal blocks in the Schur complements of block tridiagonal block Toeplitz systems discretizing bi-dimensional elliptic equations.

The paper is organized as follows. In Section 2 we provide some preliminary results including the main properties of CR, its functional interpretation, and the definitions of k -quasiseparable matrices and of hierarchical k -quasiseparable matrices. Section 3 concerns the analysis of the properties of the matrix coefficients in the Laurent expansion of the matrix function $\psi(z) = \varphi(z)^{-1}$, where $\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1$. In fact, this matrix function captures the structural and computational properties of CR. Its domain of analyticity is the annulus \mathbb{A}_t whose width has been used in [9] to prove the exponential decay. The main result of this section is Lemma 3.2 where we show that any off-diagonal block of $\psi(z)$ can be written as the sum of 4 terms; each term is the product of a Krylov matrix and of a transposed Krylov matrix.

In Section 4 —relying on a result by B. Beckermann— we provide a bound to the singular values of a matrix which satisfies a suitable displacement equation. Then we apply this result to find sharp bounds to the singular values of the off-diagonal blocks of $\psi^{(h)}(z)$ and we extend these bounds to the block $A_i^{(h)}$ and to the limit value $\lim \psi^{(h)}(z) = A_0^{(\infty)}$. The main results of this section are given in Theorems 4.6 and 4.7.

Section 5 deals with the experimental validation of the theoretical bounds to the decay. In Section 6 we show applications of the quasiseparable CR to solving block tridiagonal block Toeplitz systems and to solving certain generalized Sylvester equations. We report also the results of some numerical experiments where the above applications are tested. Finally, Section 7 draws the conclusions.

2 Some preliminaries

Throughout, \mathbb{Z} and \mathbb{N} denote the set of relative integers and of natural numbers, respectively, while \mathbb{R} and \mathbb{C} denote the complex and the real field, respectively. We recall the fundamental properties of CR and of quasiseparable matrices.

Cyclic reduction can be formulated in functional form in terms of two matrix Laurent series $\varphi(z)$ and $\psi(z)$, namely,

$$\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1, \quad \psi(z) = \varphi(z)^{-1},$$

where $\psi(z)$ is defined in the set where $\varphi(z)$ is invertible. Here and hereafter, we assume that $\varphi(z)$

is invertible in the annulus $\mathbb{A}_t = \{z \in \mathbb{C} : t \leq |z| \leq t^{-1}\}$ for some $0 < t < 1$. This assumption is generally verified in the applications. In certain cases, by means of scaling the matrices A_1 and A_{-1} by suitable constants α and α^{-1} , respectively, one can meet this assumption. Throughout we denote $\mathbb{T} = \mathbb{A}_1$ the unit circle in the complex plane.

We recall the following property which is fundamental for our analysis, see for instance [8] and [9].

Proposition 2.1. *Let A_{-1}, A_0, A_1 be $n \times n$ matrices such that CR can be carried out. Define $\varphi_h(z) = z^{-1}A_{-1}^{(h)} + A_0^{(h)} + zA_1^{(h)}$, where $A_i^{(h)}$ are the matrices generated by (1), and set $\psi_h(z) = \varphi_h(z)^{-1}$. Then*

$$\psi^{(h)}(z^{2^h}) = \frac{1}{2^h} \sum_{j=1}^{2^h} \psi(\xi_{2^h}^j z)$$

where ξ_{2^h} is a primitive 2^h -th root of the unity.

The following definitions are fundamental to formalize the fast decay of the singular values of the off-diagonal submatrices generated by CR. We say that an $m \times m$ matrix A is k -quasiseparable if all the submatrices contained in the strict upper triangular part or in the strict lower triangular part have rank at most k and there exists at least one submatrix with rank k . We say also that k is the *quasiseparable rank* of A .

We say that A is *hierarchically k -quasiseparable* if either $m \leq k$ or there exists a 2×2 block partitioning of the matrix such that the diagonal blocks are square and have size $\lfloor \frac{m}{2} \rfloor$ and $\lceil \frac{m}{2} \rceil$, respectively, the off-diagonal blocks have rank at most k and the diagonal blocks are hierarchically k -quasiseparable. Moreover, in this recursive partitioning there exists an off-diagonal submatrix of rank exactly k .

This partitioning leads to the simplest hierarchical representation, known in the literature as *hierarchically off-diagonal low rank* (HODLR), which is the one exploited in [9] for speeding up CR.

The following result states that if the singular values of the off-diagonal blocks of A decay *fast*, then A is close to a hierarchical quasiseparable matrix. That is, for a relatively small k there is a perturbation δA of *small* norm such that $A + \delta A$ is hierarchically k -quasiseparable.

Theorem 2.2. *Let $f(l)$ be a function over the positive integers, and let $A \in \mathbb{C}^{m \times m}$ be a matrix such that $\sigma_l(B) \leq f(l)$ for every off-diagonal block B in A . Then, for any l there exists a perturbation matrix δA such that $A + \delta A$ is hierarchical quasiseparable of rank at most l and $\|\delta A\|_2 \leq f(l) \cdot \log_2 m$.*

Proof. First, recall that if the nonzero singular values of a matrix B are $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k$ then, for any $j \leq k$ we may write B as a matrix of rank j plus a perturbation δB such that $\|\delta B\|_2 = \sigma_{j+1}$. Now consider an HODLR like partitioning of A with minimal blocks of dimension l . Notice that the depth of this recursive partition is $\sigma = \lceil \log_2(\frac{m}{l}) \rceil$. This way, for each off-diagonal block B of this partitioning and for any integer j , there exists a perturbation matrix that makes this block of rank j . The 2-norm of this perturbation is equal to $\sigma_{j+1}(B) \leq f(j+1)$. We may form the matrix δA which collects all these perturbations of each off-diagonal block of the above partitioning. This way, if $j = l - 1$, the off-diagonal blocks of $A + \delta A$ have rank at most l . We can now show that $\|\delta A\|_2 \leq f(l) \cdot \log_2 m$. We have

$$\delta A = \sum_{i=0}^{\sigma} \delta A_i, \quad \sigma \leq \log_2 m,$$

where δA_i is the correction obtained by putting together all the blocks at level i of subdivision, that is,

$$\delta A_0 = \begin{bmatrix} 0 & \delta X_1^{(0)} \\ \delta X_2^{(0)} & 0 \end{bmatrix}, \quad \delta A_1 = \left[\begin{array}{cc|cc} 0 & \delta X_1^{(1)} & & \\ \delta X_2^{(1)} & 0 & & \\ \hline & & 0 & \delta X_3^{(1)} \\ & & \delta X_4^{(1)} & 0 \end{array} \right], \quad \dots$$

Since the summands are just permutations of block diagonal matrices their 2-norm is the maximum of the 2-norms of the (block) diagonal entries, and this gives the desired bound. \square

Thus, our aim is to prove that the matrix function $\psi^{(h)}(z)$ defined in Proposition 2.1, has off-diagonal blocks with singular values which decay *exponentially* to zero so that the assumptions of Theorem 2.2 are satisfied with $f(l) = e^{-\alpha l}$ for some positive α . This decay property is then extended to $\varphi_h(z)$ by inversion and finally to the blocks $A_{-1}^{(h)}, A_0^{(h)}, A_1^{(h)}$ by means of interpolation. More details on this technique are given in [9].

The estimates of the parameter α given in the paper [9] depend on the value t which defines the domain \mathbb{A}_t of invertibility of the matrix $\varphi(z)$. If t gets close to 1, then α takes values close to 0, and the theoretical bound of the exponential decay loses its sharpness. Here, we introduce a different analysis which better fits with the decay observed in the numerical experiments.

We define the following class of problems for which the matrices $A_i^{(h)}$, $i = -1, 0, 1$ generated by CR through (1) have the exponential decay of the singular values in their off-diagonal blocks at any step h of the iteration.

Definition 2.3. Let $\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1$, where A_{-1}, A_0, A_1 are $m \times m$ matrices with entries in \mathbb{C} , be such that CR can be applied with no breakdown by means of (1). Let $f(l)$ be a positive function in $l^1(\mathbb{N})$. We say that $\varphi(z)$ is *f-decaying-quasiseparable* if, $\forall h \in \mathbb{N}$, $\forall z \in \mathbb{T}$ and for every off-diagonal block $\tilde{C}^{(h)}(z)$ of $\psi^{(h)}(z)$, we have

$$\sigma_l(\tilde{C}^{(h)}(z)) \leq \|\psi^{(h)}(z)\|_2 \cdot f(l),$$

where $\sigma_l(\tilde{C}^{(h)}(z))$ denotes the l -th singular value of the matrix $\tilde{C}^{(h)}(z)$. We define the set of such matrix functions $\varphi(z)$ as $\text{DQ}(f)$.

3 Laurent coefficients of an off-diagonal block

In this section, we consider the matrix Laurent series expansion of $\psi(z)$, that is, $\psi(z) = \sum_{i=-\infty}^{+\infty} z^i H_i$ for $z \in \mathbb{A}_t$, which exists and is convergent since $\psi(z)$ is analytic in the domain \mathbb{A}_t where $\varphi(z)$ is analytic and non-singular. Then we will analyze the properties of the coefficients of an off-diagonal block of this Laurent series.

We define the eigenvalues of $\varphi(z)$ as the roots of the polynomial $p(z) = \det(A_{-1} + zA_0 + z^2A_1)$. Observe that if $\det A_1 \neq 0$ the polynomial $p(z)$ has degree $d = 2m$ so that there are $2m$ roots. If, on the other hand, $\det A_1 = 0$ then $d < 2m$ and for this reason, we add to the d roots of $p(z)$ other $2m - d$ roots at the infinity. In this way we can say that $\varphi(z)$ has always $2m$ eigenvalues including possible eigenvalues at the infinity.

Here we assume that the eigenvalues ξ_i , $i = 1, \dots, 2m$ of $\varphi(z)$ satisfy the balanced splitting property with respect to the unit circle

$$|\xi_1| \leq \dots \leq |\xi_m| < t < 1 < t^{-1} < |\xi_{m+1}| \leq \dots \leq |\xi_{2m}|. \quad (2)$$

We call t the radius of the splitting. The splitting property (2) is needed to guarantee the applicability of CR and that the convergence to zero of the blocks $A_{-1}^{(h)}$ and $A_1^{(h)}$ is doubly exponential [8].

Consider the following partitioning of $\psi(z)$ and $\varphi(z)$

$$\varphi(z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix}, \quad \psi(z) = \begin{pmatrix} \tilde{A}(z) & \tilde{B}(z) \\ \tilde{C}(z) & \tilde{D}(z) \end{pmatrix} = \begin{pmatrix} S_D(z)^{-1} & * \\ -D(z)^{-1}C(z)S_D(z)^{-1} & * \end{pmatrix},$$

where the diagonal blocks are square, $S_D(z) = A(z) - B(z)D(z)^{-1}C(z)$ is the Schur complement of $D(z)$, and $*$ denotes blocks which are not relevant for our analysis.

Moreover, suppose that the splitting (2) holds also for the eigenvalues of $D(z)$ –this is true for problems from stochastic models which are ruled by M-matrices– and assume that the matrix coefficients A_i have quasiseparable rank k for $i = -1, 0, 1$. These hypotheses are always satisfied for a large class of important problems like not null recurrent Quasi Birth-Death problems (QBDs) with banded blocks, up to rescaling the coefficients [8]. This guarantees that the matrix functions $\varphi(z)$ and $D(z)$ are invertible in the annulus \mathbb{A}_t for some $t < 1$.

Observe that, since the off-diagonal blocks of A_i have rank at most k for $i = -1, 0, 1$, then any off-diagonal block $C(z)$ of $\varphi(z)$ can be written as

$$C(z) = z^{-1}U_{-1}V_{-1}^t + U_0V_0^t + zU_1V_1^t, \quad \|U_i\| = \|A_i\|, \quad \|V_i\| = 1,$$

where U_i and V_i have k columns and the superscript t denotes transposition.

Defining

$$U = [U_{-1} \mid U_0 \mid U_1], \quad V(z) = [z^{-1}V_{-1} \mid V_0 \mid zV_1],$$

we can write $\tilde{C}(z) = -\tilde{U}(z)\tilde{V}(z)^t$, where $\tilde{U}(z) = D(z)^{-1}U$ and $\tilde{V}(z) = S_D(z)^{-t}V(z)$. Observe that $S_D(z)^{-1}$ is the upper left diagonal block of $\psi(z)$. This gives us a crucial information on the coefficients of the matrix Laurent series expansion of $D(z)^{-1}$ and $S_D(z)^{-1}$. In order to perform this analysis we have to recall a general result which provides an explicit expression of the coefficients H_i of the Laurent expansion of $\psi(z)$.

Theorem 3.1 (Part of Theorem 3.20 in [8]). *Let $\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1$ with $A_i \in \mathbb{R}^{m \times m}$, $i = -1, 0, 1$ and assume that the eigenvalues ξ_i , $i = 1, \dots, 2m$ of $\varphi(z)$ satisfy (2). Moreover suppose that there exist R and \hat{R} with spectral radius less than 1 which solve the matrix equations*

$$A_1 + XA_0 + X^2A_{-1} = 0, \tag{3}$$

$$X^2A_1 + XA_0 + A_{-1} = 0, \tag{4}$$

respectively. Then there exist G and \hat{G} solutions of the reversed matrix equations

$$A_1X^2 + A_0X + A_{-1} = 0, \tag{5}$$

$$A_1 + A_0X + A_{-1}X^2 = 0, \tag{6}$$

respectively, with spectral radius less than 1. Moreover, expanding $\varphi(z)^{-1} = \sum_{j=-\infty}^{+\infty} z^j H_j$ yields

$$H_j = \begin{cases} H_0 \hat{R}^{-j} = G^{-j} H_0 & j \leq 0 \\ H_0 R^j = \hat{G}^j H_0 & j \geq 0 \end{cases}, \quad G = H_{-1} H_0^{-1}, \quad \hat{G} = H_1 H_0^{-1}, \quad R = H_0^{-1} H_1, \quad \hat{R} = H_0^{-1} H_{-1}.$$

The spectrum of G and \hat{R} is formed by the eigenvalues of $\varphi(z)$ inside the unit disc, the spectrum of \hat{G} and R is formed by the reciprocals of the eigenvalues of $\varphi(z)$ outside the unit disc.

This result, applied with $\varphi(z) = D(z)$ and combined with what said previously, tells us that the Laurent coefficients of $\tilde{U}(z)$ are of the form

$$D^{-1}(z) = \sum_{j \in \mathbb{Z}} z^j H_{D,j}, \quad H_{D,j} = \begin{cases} G_D^{-j} H_{D,0} & j \leq 0, \\ \widehat{G}_D^j H_{D,0} & j \geq 0, \end{cases}$$

where G_D and \widehat{G}_D are the solutions of the matrix equations associated with $D(z)$ of the kind (5) and

$$S_D(z)^{-1} = \sum_{j \in \mathbb{Z}} z^j H_{S,j}, \quad H_{S,j} = \begin{cases} [I \ 0] H_0 \widehat{R}^{-j} [I \ 0]^t & j \leq 0, \\ [I \ 0] H_0 R^j [I \ 0]^t & j \geq 0, \end{cases}$$

where the latter equation is obtained by applying Theorem 3.1 to the original matrix Laurent polynomial $\varphi(z)$.

Consider the simpler case where $k = 1$ and the decomposition of each off-diagonal block $C(z)$ of $\varphi(z)$ can be written as $C(z) = uv^t$ (a constant dyad). This is not restrictive since, in the other cases, we can write $C(z)$ as a linear combination of at most $3k$ terms of the above form with coefficients z^j , $j = -1, 0, 1$.

In view of Theorem 3.1, for $z \in \mathbb{T}$ we can write each off-diagonal block $\tilde{C}(z)$ of $\psi(z)$ as

$$\tilde{C}(z) = \tilde{u}(z) \tilde{v}(z)^t, \quad \tilde{u}(z) = \sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u z^j + \sum_{j < 0} G_D^{-j} H_{D,0} u z^j,$$

where $\tilde{v}(z) = S_D(z)^{-t} v$, the matrix function $S_D(z)^{-1}$ is the inverse of the Schur complement of $D(z)$ and $\|v\|_2 \leq 1$. Observe that the Laurent coefficients of $\tilde{u}(z)$ corresponding to positive powers of z lie in the Krylov subspace $\mathcal{K}_j(\widehat{G}_D, H_{D,0}u)$, while the coefficients corresponding to the negative powers are in $\mathcal{K}_j(G_D, H_{D,0}u)$. Here we denote by $\mathcal{K}_j(A, v)$ the $(j+1)$ -dimensional Krylov subspace

$$\mathcal{K}_j(A, v) = \text{span}(v, Av, A^2v, \dots, A^jv).$$

Analogously we know that

$$v^t S_D(z)^{-1} = \left(\sum_{j \geq 0} \widehat{v}^t H_{\psi,0} R^j z^j + \sum_{j < 0} \widehat{v}^t H_{\psi,0} \widehat{R}^{-j} z^j \right) \begin{bmatrix} I \\ 0 \end{bmatrix}, \quad \widehat{v} := \begin{bmatrix} v \\ 0 \end{bmatrix},$$

therefore

$$\begin{aligned} -\tilde{C}(z) &= \left(\sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u z^j + \sum_{j < 0} G_D^{-j} H_{D,0} u z^j \right) \\ &\quad \cdot \left(\sum_{j > 0} \widehat{v}^t H_{\psi,0} R^j z^j + \sum_{j \leq 0} \widehat{v}^t H_{\psi,0} \widehat{R}^{-j} z^j \right) \begin{bmatrix} I \\ 0 \end{bmatrix}. \end{aligned} \tag{7}$$

Denoting by $\tilde{C}^{(h)}(z^{2^h})$ the corresponding off-diagonal sub-block in $\psi^{(h)}$, from Proposition 2.1 we have

$$\tilde{C}^{(h)}(z^{2^h}) = \frac{1}{2^h} \sum_{j=1}^{2^h} \tilde{C}(z \zeta_{2^h}^j). \tag{8}$$

In the following, the matrices with columns of the form $A^j b$, for some matrix A and a vector b , which we call *Krylov matrices*, will play an important role. We indicate a Krylov matrix with the notation

$$\mathcal{KM}_n(A, b) := [b \mid Ab \mid \dots \mid A^{n-1}b].$$

Moreover, we denote by J the counter-identity matrix of appropriate size such that $[1, 2, \dots, n]J = [n, n-1, \dots, 1]$.

Relying on (7) we can prove the following result.

Lemma 3.2. *If $C(z) = uv^t$, then $-\tilde{C}^{(h)}(z^{2^h})$ is the sum of the following four outer products:*

$$\begin{aligned} -\tilde{C}^{(h)}(z^{2^h}) &= \left[\mathcal{KM}_{2^h}(\widehat{G}_D, \widehat{a}) \cdot \mathcal{KM}_{2^h}(\widehat{R}^t, \widehat{b})^t \right. \\ &\quad + z^{2^h-1} \cdot \mathcal{KM}_{2^h}(\widehat{G}_D, \widehat{a}) \cdot J \cdot \mathcal{KM}_{2^h}(R^t, b)^t \\ &\quad + z^{1-2^h} \cdot \mathcal{KM}_{2^h}(G_D, a) \cdot J \cdot \mathcal{KM}_{2^h}(\widehat{R}^t, \widehat{b})^t \\ &\quad \left. + \mathcal{KM}_{2^h}(G_D, a) \cdot \mathcal{KM}_{2^h}(R^t, b)^t \right] \begin{bmatrix} I \\ 0 \end{bmatrix}, \end{aligned} \tag{9}$$

where

$$\begin{aligned} a &= \left(\sum_{s \in 2^h \mathbb{Z} \cap \mathbb{N}} z^{-s-1} G_D^{s+1} \right) H_{D,0} u, & b &= \left(\sum_{s \in 2^h \mathbb{Z} \cap \mathbb{N}} z^{s+1} R^{s+1} \right)^t H_{\psi,0}^t \widehat{v}, \\ \widehat{a} &= \left(\sum_{s \in 2^h \mathbb{Z} \cap \mathbb{N}} z^s \widehat{G}_D^s \right) H_{D,0} u, & \widehat{b} &= \left(\sum_{s \in 2^h \mathbb{Z} \cap \mathbb{N}} z^{-s} \widehat{R}^s \right)^t H_{\psi,0}^t \widehat{v}. \end{aligned}$$

Proof. Thanks to (7) we may write $-\tilde{C}(z)$ as the sum of four outer products. By the linearity of (8) we can consider them separately. Take for example

$$\left(\sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u z^j \right) \cdot \left(\sum_{j \leq 0} \widehat{v}^t H_{\psi,0} \widehat{R}^{-j} z^j \right) = \sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u \widehat{v}^t H_{\psi,0} \sum_{s \geq 0} \widehat{R}^s z^{j-s},$$

where we have ignored $[I \ 0]^t$ because it can be factored on the right. The block $\tilde{C}^{(h)}(z)$ of $\psi^{(h)}(z)$ corresponding to $\tilde{C}(z)$ in $\psi(z)$ verifies the relation $\tilde{C}^{(h)}(z^{2^h}) = \frac{1}{2^h} \sum_{l=1}^{2^h} \tilde{C}(z \zeta_{2^h}^l)$ so that

$$\begin{aligned} \frac{1}{2^h} \sum_{l=1}^{2^h} \sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u \widehat{v}^t H_{\psi,0} \sum_{s \geq 0} \widehat{R}^s (z \zeta_{2^h}^l)^{j-s} &= \sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u \widehat{v}^t H_{\psi,0} \sum_{s \in (2^h \mathbb{Z} + j) \cap \mathbb{N}} \widehat{R}^s z^{j-s} \\ &= \sum_{j=0}^{2^h-1} \left(\sum_{s \in (2^h \mathbb{Z} + j) \cap \mathbb{N}} z^s \widehat{G}_D^s \right) H_{D,0} u \widehat{v}^t H_{\psi,0} \left(\sum_{s \in (2^h \mathbb{Z} + j) \cap \mathbb{N}} \widehat{R}^s z^{-s} \right), \end{aligned}$$

where $2^h \mathbb{Z} + j := \{s \in \mathbb{Z} \mid s \equiv j \pmod{2^h}\}$. Observe that the $(j+1)$ -st term of the previous sum is equal to the j -th term multiplied on the left by $z \widehat{G}_D$ and on the right by $z^{-1} \widehat{R}$. In particular we can rewrite it as

$$\left[a \mid z \widehat{G}_D \cdot a \mid \dots \mid (z \widehat{G}_D)^{2^h-1} \cdot a \right] \cdot \left[\widehat{b} \mid (z^{-1} \widehat{R}^t) \cdot \widehat{b} \mid \dots \mid (z^{-1} \widehat{R}^t)^{2^h-1} \cdot \widehat{b} \right]^t,$$

that is, $\mathcal{KM}_{2^h}(z\widehat{G}_D, a) \cdot \mathcal{KM}_{2^h}(z^{-1}\widehat{R}^t, \widehat{b})$.

The variables z in the above factors cancel out, and we obtain one of the addends in the statement of the theorem.

Then consider $\left(\sum_{j \geq 0} \widehat{G}_D^j H_{D,0} u z^j\right) \cdot \left(\sum_{j > 0} \widehat{v}^t H_{\psi,0} R^{-j} z^j\right)$ for which we arrive at the expression

$$\sum_{j=0}^{2^h-1} \left(\sum_{s \in (2^h \mathbb{Z} + j) \cap \mathbb{N}} z^s \widehat{G}_D^s \right) H_{D,0} u \widehat{v}^t H_{\psi,0} \left(\sum_{s \in (2^h \mathbb{Z} - j) \cap \mathbb{N}} R^s z^s \right).$$

This time we have a product of the form

$$\left[a \mid z\widehat{G}_D \cdot a \mid \dots \mid (z\widehat{G}_D)^{2^h-1} \cdot a \right] \cdot \left[(zR^t)^{2^h-1} \cdot b \mid \dots \mid (zR^t) \cdot b \mid b \right]^t,$$

that is $z^{2^h-1} \cdot \mathcal{KM}_{2^h}(\widehat{G}_D, a) \cdot J \cdot \mathcal{KM}_{2^h}(\widehat{R}^t, \widehat{b})$. The other two relations are obtained in a similar manner. \square

In the case $C(z) = z^s u v^t$ with $s = -1, 1$ one can recover the same behavior just taking into account a shift in the powers of z in (7) that modifies the powers of z in the outer products accordingly.

4 Singular values and displacement rank

Lemma 3.2 provides a tool for analyzing the singular values decay of the off-diagonal block $\widetilde{C}^{(h)}(z)$ of $\psi^{(h)}(z)$. In fact, these blocks can be written as the sum of few terms each of them is the product of two Krylov matrices, one of which is transposed.

The next step is to investigate the singular values of a product of this kind. In this analysis, we rely on the concept of displacement rank and on some result by B. Beckermann [3], of which we report the proof.

Definition 4.1. Given matrices $A, B, X \in \mathbb{C}^{m \times m}$ the *displacement rank* of X with respect to the pair (A, B) is defined as

$$\rho_{A,B}(X) = \text{rank}(AX - XB).$$

We need also to introduce the set $\mathcal{R}_{n,d}$ of rational functions over \mathbb{C} where n and d are the degree of the numerator and of the denominator, respectively.

For a matrix X with a small displacement rank it is possible to provide bounds on its singular values in terms of the optimal values of some Zolotarev problems [29] according to the following result of B. Beckermann [3].

Theorem 4.2. Let $X \in \mathbb{C}^{m \times m}$ and suppose that there exist two normal matrices $A, B \in \mathbb{C}^{m \times m}$ such that $\rho_{A,B}(X) = d$. Then, indicating with E and F the spectrum of A and B respectively, for the singular values $\sigma_i(X)$ of X it holds:

$$\frac{\sigma_{1+l \cdot d}(X)}{\|X\|_2} \leq Z_l(E, F) := \inf_{r(x) \in \mathcal{R}_{l,l}} \frac{\max_{x \in E} |r(x)|}{\min_{x \in F} |r(x)|}, \quad l = 1, 2, \dots$$

Proof. Consider $p(x) := \sum_{i=0}^l p_i x^i$ and $q(x) := \sum_{i=0}^l q_i x^i$ polynomials of degree l and define $r(x) := \frac{p(x)}{q(x)}$. We prove that the matrix

$$\Delta := q(A)Xp(B) - p(A)Xq(B)$$

has rank at most $l \cdot d$. Without loss of generality we consider the case $d = 1$ and suppose $AX - XB = uv^t$. We can prove by induction that $A^k X - XB^k = \sum_{h=0}^{k-1} A^h uv^t B^{k-1-h}$. For $k = 1$ the property trivially holds. For $k > 1$ one has:

$$\begin{aligned} A^k X &= A^{k-1} XB + A^{k-1} uv^t = XB^k + \left(\sum_{h=0}^{k-2} A^h uv^t B^{k-1-h} \right) B + A^{k-1} uv^t \\ &= XB^k + \sum_{h=0}^{k-1} A^h uv^t B^{k-1-h}. \end{aligned}$$

Now, observe that

$$\Delta = q(A)Xp(B) - p(A)Xq(B) = \sum_{i \neq j}^d (q_i p_j - q_j p_i) (A^i X B^j - A^j X B^i),$$

and if $i > j$ (the other case is analogous)

$$A^i X B^j - A^j X B^i = A^j (A^{i-j} X - X B^{i-j}) B^j = A^j \left(\sum_{h=0}^{i-j-1} A^h uv^t B^{k-1-h} \right) B^j.$$

In particular all the addends involved in the expansion of Δ can be expressed as sum of dyads whose left vectors belong to the Krylov space $\mathcal{K}_l(A, u)$ and so it has rank at most l .

Assume that $q(A)$ and $p(B)$ are invertible, define $Y := q(A)^{-1} \Delta p(B)^{-1}$ observe that $X - Y = r(A)Xr(B)^{-1}$ so that

$$\|X - Y\|_2 = \|r(A)Xr(B)^{-1}\|_2 \leq \|X\|_2 \max_E |r(x)| \max_F |r(x)|^{-1} = \|X\|_2 \frac{\max_E |r(x)|}{\min_F |r(x)|}.$$

Since $\sigma_{k+1}(X)$ coincides with the minimum of $\|X - W\|_2$ taken over all the matrices W of rank k , and since $\text{rank}(Y) = \text{rank}(\Delta) \leq l \cdot d$, we find that

$$\sigma_{l \cdot d + 1}(X) \leq \|X - Y\|_2 \leq \|X\|_2 \frac{\max_E |r(x)|}{\min_F |r(x)|}.$$

Taking the infimum over the set of rational functions of degree (d, d) completes the proof. \square

Note that the normality hypothesis can be relaxed by replacing it with the diagonalizability of A and B . The price to pay is a larger constant depending on the conditioning of the eigenvector matrices as stated by the following

Corollary 4.3. *Let $X \in \mathbb{C}^{m \times m}$ and suppose that there exist two diagonalizable matrices $A, B \in \mathbb{C}^{m \times m}$ such that $\Delta_{A,B}(X) = d$, that is $A = V_A D_A V_A^{-1}$, $B = V_B D_B V_B^{-1}$ with D_A and D_B diagonal matrices. Then, indicating with E and F the spectrum of A and B respectively, it holds:*

$$\sigma_{1+l \cdot d}(X) \leq Z_l(E, F) \cdot \|X\|_2 \cdot \kappa(V_A) \cdot \kappa(V_B)$$

where $\kappa(W) = \|W\|_2 \|W^{-1}\|_2$ denotes the spectral condition number of W .

The case where E and F are disjoint subsets of the real line, has been extensively studied by Zolotarev [29] who managed to provide explicit bounds for $Z_l(E, F)$. The result we are going to quote is adapted to our case and can be found in [15]. See also [1, 2, 22] for more classical references.

Theorem 4.4 (Zolotarev). *Let $\delta \in (0, 1)$, $E := [-\infty, -\delta^{-1}] \cup [\delta^{-1}, +\infty]$ and $F = [-\delta, \delta]$. Then*

$$Z_{2l}(E, F) \leq \frac{2\rho^l}{1 - 2\rho^l},$$

where

$$\rho := \exp\left(-\frac{\pi K(\sqrt{1 - \delta^4})}{2K(\delta^2)}\right), \quad K(x) := \int_0^1 \frac{1}{\sqrt{(1-t^2)(1-x^2t^2)}} dt.$$

Moreover, if $\delta \approx 1$ then $K(\delta^2) \approx \log\left(\frac{4}{\sqrt{1-\delta^4}}\right)$ and $K(\sqrt{1-\delta^4}) \approx \frac{\pi}{2}$, yielding

$$Z_{2l}(E, F) \leq \frac{2\rho^l}{1 - 2\rho^l} \approx \frac{2\tilde{\rho}^l}{1 - 2\tilde{\rho}^l}, \quad \tilde{\rho} := \exp\left(-\frac{\pi^2}{2 \log\left(\frac{16}{1-\delta^4}\right)}\right).$$

Now, we prove that some matrices involved in the decomposition of the off-diagonal submatrices of $\psi^{(h)}(z)$ enjoy a small displacement rank.

Proposition 4.5. *Under the assumptions and the notation of Lemma 3.2 we have*

$$\tilde{C}^{(h)}(z^{2^h}) = [I \ I] \cdot X^{(h)}(z) Y^{(h)}(z)^t \cdot [I \ I]^t \cdot [I \ 0]^t$$

where

$$X^{(h)}(z) := \begin{bmatrix} \mathcal{K}\mathcal{M}_{2^h}(\widehat{G}_D, \widehat{a}) \\ z^{1-2^h} \mathcal{K}\mathcal{M}_{2^h}(G_D, a)J \end{bmatrix}, \quad Y^{(h)}(z) := \begin{bmatrix} z^{2^h-1} \mathcal{K}\mathcal{M}_{2^h}(R^t, b)J \\ \mathcal{K}\mathcal{M}_{2^h}(\widehat{R}^t, \widehat{b}) \end{bmatrix}.$$

Moreover, we have the following displacement relations:

$$\rho_{W_D, \Pi}(X^{(h)}) = 1, \quad \rho_{W, \Pi}(Y^{(h)}) = 1,$$

with

$$W_D := \begin{bmatrix} \widehat{G}_D & 0 \\ 0 & G_D^\dagger \end{bmatrix}, \quad W := \begin{bmatrix} (R^\dagger)^t & 0 \\ 0 & \widehat{R}^t \end{bmatrix}, \quad \Pi = \begin{bmatrix} 0 & & & 1 \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & & 1 & 0 \end{bmatrix},$$

where the super-script \dagger indicates the Moore-Penrose pseudoinverse.

Proof. The first claim simply follows by expanding the expression for $\tilde{C}^{(h)}(z^{2^h})$ and by comparing it with equation (9). Concerning the displacement equations, a direct computation shows that the matrices

$$W_D X^{(h)}(z) - X^{(h)}(z) \Pi \quad \text{and} \quad W Y^{(h)}(z) - Y^{(h)}(z) \Pi$$

have only the last column possibly different from zero. \square

The above result allows us to give a bound to the singular values of $\tilde{C}^{(h)}(z)$.

Theorem 4.6. *Let $\varphi(z) = z^{-1}A_{-1} + A_0 + zA_1$ be an $m \times m$ matrix Laurent polynomial such that the CR —given by (1)— can be carried out with no breakdown, the splitting property (2) is verified, and $\varphi(z)$ has quasiseparable rank 1 for every $z \in \mathbb{T}$. Assume that the matrices R and \widehat{R} which solve the matrix equations (3) are diagonalizable by means of the two eigenvector matrices V_R and $V_{\widehat{R}}$, respectively. Assume that G_D and R are invertible. Then $\varphi(z) \in \text{DQ}(f)$ where*

$$f(l) := \gamma \cdot Z_l(E, \mathbb{T}),$$

with γ a multiple of $\max\{\kappa(V_R), \kappa(V_{\widehat{R}})\}$ and E contains the eigenvalues of $\varphi(z)$.

Proof. Notice that a generic off-diagonal matrix $\widetilde{C}^{(h)}(z)$ in $\psi^{(h)}(z)$ can be seen as a submatrix of

$$[I \ I]X^{(h)}(z)Y^{(h)}(z)^t \begin{bmatrix} I \\ I \end{bmatrix}.$$

In view of Proposition 4.5 we know that $Y^{(h)}(z)$ has displacement rank 1. The displacement relation for $Y^{(h)}(z)$ involves the matrices W and Π whose eigenvalues correspond to those of $\varphi(z)$ and to the roots of the unity of order 2^h , respectively. Moreover, W is diagonalizable by means of $V_W := \text{diag}(V_R^{-t}, V_{\widehat{R}}^{-t})$. Therefore, applying Corollary 4.3 we can write

$$\sigma_{1+l}(Y^{(h)}(z)) \leq Z_l(E, \mathbb{T}) \cdot \|Y^{(h)}(z)\|_2 \cdot \kappa(V_W).$$

Since W is block-diagonal we have $\kappa(V_W) = \max\{\kappa(V_R), \kappa(V_{\widehat{R}})\}$. In particular we can bound the singular values of $\widetilde{C}^{(h)}(z)$ with the quantity

$$\sigma_{1+l}(\widetilde{C}^{(h)}(z)) \leq 2 \cdot Z_l(E, \mathbb{T}) \cdot \|X^{(h)}(z)\|_2 \cdot \|Y^{(h)}(z)\|_2 \cdot \kappa(V_W).$$

Defining $\gamma := 2 \cdot \kappa(V_W) \cdot \max_{h \in \mathbb{N}, z \in \mathbb{T}} \frac{2\|X^{(h)}(z)\|_2 \cdot \|Y^{(h)}(z)\|_2}{\|\psi^{(h)}(z)\|_2}$ we get the thesis. \square

The constant γ in the previous theorem is an index of how much the factorization $X^{(h)}(z)Y^{(h)}(z)^t$ is unbalanced. This limitation is not present in the following result which describes the asymptotic behavior as $h \rightarrow \infty$. It is possible to show that the block diagonal terms in $W^{(h)}(z) = X^{(h)}(z)Y^{(h)}(z)^t$ quickly decay to 0 in practice, making the following bounds numerically accurate after a few steps.

Theorem 4.7. *Let $W^{(h)}(z) = X^{(h)}(z)Y^{(h)}(z)^t$, where $X^{(h)}(z)$ and $Y^{(h)}(z)$ are the matrices defined in Proposition 4.5. Then $\lim_{h \rightarrow \infty} W^{(h)}(z) = W^{(\infty)}$ has the following block partitioning*

$$W^{(\infty)} = \begin{bmatrix} 0 & B_1 \\ B_2 & 0 \end{bmatrix}$$

where the diagonal blocks are square and the off-diagonal blocks are independent of z . Moreover, we have $\rho_{V_D, V}(W^{(\infty)}) = 2$, where

$$V_D := \begin{bmatrix} \widehat{G}_D & 0 \\ 0 & G_D \end{bmatrix} \quad \text{and} \quad V := \begin{bmatrix} R^\dagger & 0 \\ 0 & \widehat{R}^\dagger \end{bmatrix}.$$

If the matrices G_D, \widehat{G}_D, R and \widehat{R} are diagonalizable by means of $V_{G_D}, V_{\widehat{G}_D}, V_R$ and $V_{\widehat{R}}$, respectively, then, indicating with \widetilde{C} the off-diagonal block in $H_{\psi, 0}$ corresponding to $\widetilde{C}(z)$ we have the following bounds to its singular values

$$\sigma_{1+2l}(\widetilde{C}) \leq \gamma \cdot Z_l(E, F), \quad \gamma := 2 \cdot \max\{\kappa(V_G), \kappa(V_{\widehat{G}})\} \cdot \max\{\kappa(V_R), \kappa(V_{\widehat{R}})\} \cdot \|\widetilde{C}\|_2,$$

where E contains the eigenvalues of $\varphi(z)$ and $D(z)$ inside the unit disc while F contains those outside.

Proof. From the definition of $X^{(h)}$ and $Y^{(h)}$ one has

$$W^{(h)}(z) = \begin{bmatrix} z^{2^h-1} \mathcal{KM}_{2^h}(\widehat{G}_D, \widehat{a}) J(\mathcal{KM}_{2^h}(R^t, b))^t & \mathcal{KM}_{2^h}(\widehat{G}_D, \widehat{a}) (\mathcal{KM}_{2^h}(\widehat{R}^t, \widehat{b}))^t \\ \mathcal{KM}_{2^h}(G_D, a) (\mathcal{KM}_{2^h}(R^t, b))^t & z^{1-2^h} \mathcal{KM}_{2^h}(G_D, a) J(\mathcal{KM}_{2^h}(\widehat{R}^t, \widehat{b}))^t. \end{bmatrix}$$

Since the spectral radii of the matrices R , \widehat{R} , G_D and \widehat{G}_D are less than 1, then the block diagonal entries of $W^{(h)}$ tend to zero as $h \rightarrow \infty$ and the two off-diagonal blocks have limits B_1 and B_2 , respectively. More precisely

$$W^{(\infty)} = \begin{bmatrix} 0 & B_1 \\ B_2 & 0 \end{bmatrix}, \quad B_1 = \sum_{i \geq 0} \widehat{G}_D^i \widehat{a} \widehat{b}^t \widehat{R}^i, \quad B_2 = \sum_{i \geq 0} G_D^i a b^t R^i.$$

Thus, we have

$$\widehat{G}_D B_1 - B_1 \widehat{R}^\dagger = \widehat{a} \widehat{b}^t \widehat{R}^\dagger.$$

An analogous argument holds for B_2 , and gives the rank-2 displacement. The matrix \widetilde{C} can be written as $\widetilde{C} = [I \ I] \cdot W^{(\infty)} \cdot [I \ I]^t \cdot [I \ 0]$, which corresponds to an off-diagonal block of $\lim_{h \rightarrow \infty} \psi^{(h)}(z)$. Due to the recurrence relation $\psi^{(h+1)}(z^2) = \frac{1}{2}(\psi^{(h)}(z) + \psi^{(h)}(-z))$, this limit is equal to the central coefficient $H_{\psi,0}$ in the series expansion of $\psi(z)$. The thesis follows by applying Corollary 4.3. \square

5 Experimental validation of the results

This section is devoted to verify the previous results by means of numerical experiments. We do that by computing numerical estimates of the bound given in Theorem 4.7 together with the singular values of the off-diagonal blocks of $H_{\psi,0}$. The actual bounds are obtained by choosing a particular family of rational functions that suit the considered problem. We will see that, even if our choices are relatively simple, and not optimal, they already provide sharp decay bounds in practice.

As a first example, we consider instances of the problem coming from the framework of Markov chains i.e., the sum $A_{-1} + A_0 + I + A_1$ is sub-stochastic, that is, it has non-negative entries and the sum along each row is at most 1. In particular, the matrices A_{-1} , $I + A_0$ and A_1 have non negative entries and are scaled in order to satisfy the splitting assumption (2) (see also Section 4.3 in [9]).

We select dense 300×300 -blocks generated at random and such that $\varphi(z)$ is of quasiseparable rank 1. For satisfying the latter hypothesis we impose that the strictly triangular parts of the blocks are the restrictions of dyads with the same left vectors.

We divide the resulting distribution of the eigenvalues in three cluster. One is contained in a neighborhood of 0, another is in the complement of the disc of radius 4 and finally we have two eigenvalues close to 1, λ_1 and λ_2 , inside and outside the unit circle, respectively.

Motivated by this, we choose the sequence of rational function

$$r_l(z) := \frac{z - \lambda_1}{z - \lambda_2} z^{l-1},$$

for roughly estimating the Zolotarev problem. The results are shown in Figure 2.

As a second example, we consider the linear system arising from the discretization of a 2D

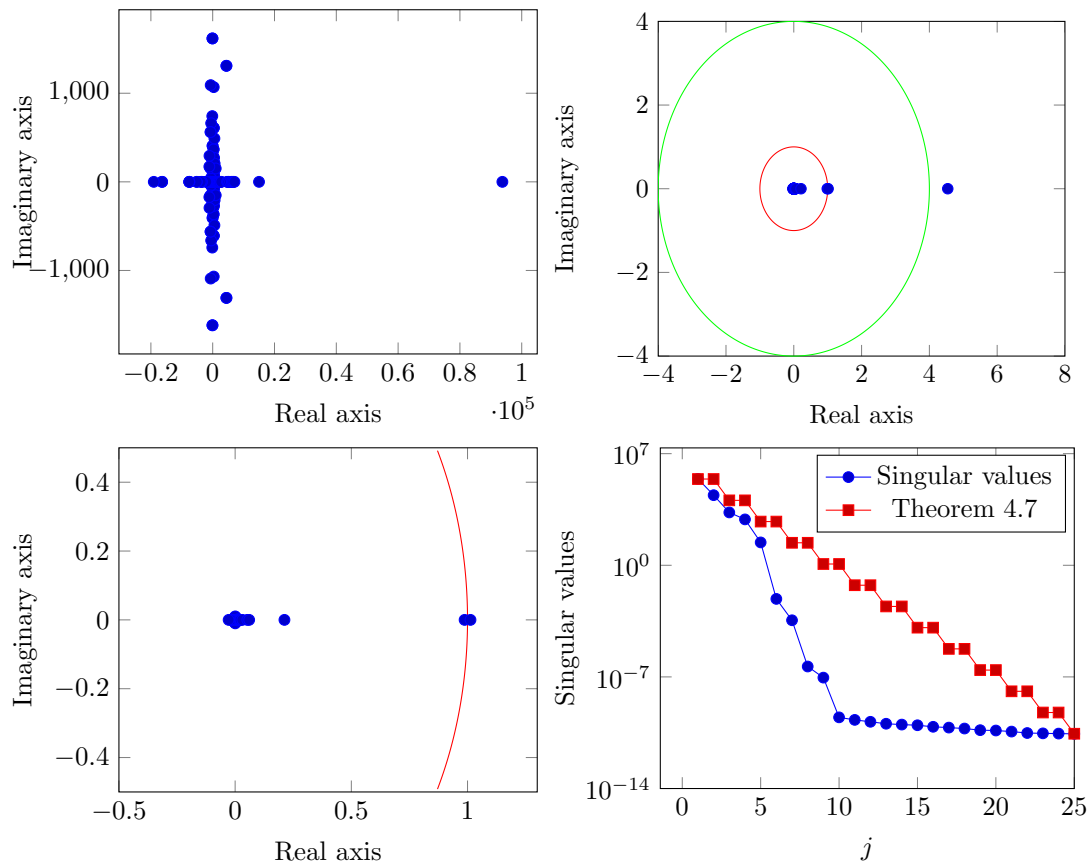


Figure 2: Singular value decay in H_0 and the bound given by Theorem 4.7.

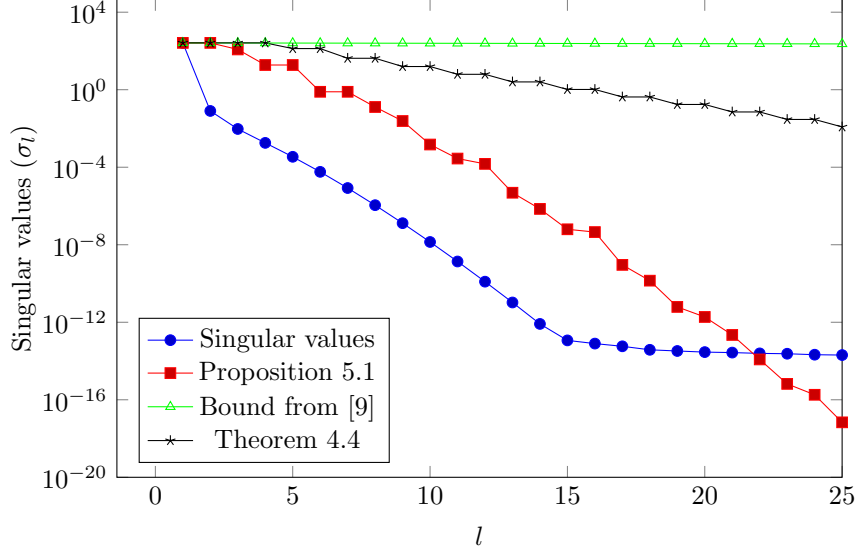


Figure 3: Decay of the singular values in one of the off-diagonal blocks of H_0 in the Laurent expansion of $\psi(z)$, computed by means of the CR for the Poisson matrix. We have reported the actual decay and the bounds obtained by means of Proposition 5.1, the results in [9], and Theorem 4.4.

A first application concerns solving a block tridiagonal linear system of the kind $\mathcal{A}_n x = b$ where $\mathcal{A}_n = \text{trid}_n(B, A, C)$, the blocks A, B, C are $m \times m$ matrices such that CR can be carried out with no breakdown, the right-hand side vector b and the unknown vector x are partitioned into n blocks b_i and x_i , respectively of size m . For simplicity, assume $n = 2^k - 1$ so that the description of CR is simpler, for more details in the general case we refer the reader to [10].

The system can be written in the form

$$\begin{bmatrix} A & C & & & \\ B & A & C & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & C \\ & & & B & A \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \\ b_n \end{bmatrix}, \quad A, B, C \in \mathbb{R}^{m \times m}, \quad x_i, b_i \in \mathbb{R}^m. \quad (10)$$

An odd-even permutation of block rows and columns yields

$$\left[\begin{array}{ccc|ccc} A & & & C & & \\ & A & & B & \ddots & \\ & & \ddots & & \ddots & C \\ & & & & \ddots & B \\ \hline B & C & & A & & \\ & & \ddots & & \ddots & \\ & & & B & C & \\ \hline & & & & & A \end{array} \right] \begin{bmatrix} x_1 \\ x_3 \\ x_5 \\ \vdots \\ x_n \\ \hline x_2 \\ \vdots \\ x_{n-1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_3 \\ b_5 \\ \vdots \\ b_n \\ \hline b_2 \\ \vdots \\ b_{n-1} \end{bmatrix}$$

Then one step of block Gaussian elimination performed to vanish the south-western block, yields

$$\left[\begin{array}{ccc|ccc} A & & & C & & \\ & A & & B & \ddots & \\ & & \ddots & & \ddots & \\ & & & & & C \\ \hline & & & A^{(1)} & C^{(1)} & \\ & & & B^{(1)} & \ddots & \\ & & & & \ddots & C^{(1)} \\ & & & & & B^{(1)} & A^{(1)} \end{array} \right] \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ \vdots \\ x_n \\ \vdots \\ \vdots \\ \vdots \\ x_{n-1} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ \vdots \\ b_n \\ b_1^{(1)} \\ b_2^{(1)} \\ \vdots \\ \vdots \\ b_{\frac{n-1}{2}}^{(1)} \end{bmatrix}$$

with

$$\begin{aligned} A^{(1)} &= A - BA^{-1}C - CA^{-1}B, \\ B^{(1)} &= -BA^{-1}B, \quad C^{(1)} = -CA^{-1}C, \\ b_i^{(1)} &= b_{2i} - BA^{-1}b_{2i-1} - CA^{-1}b_{2i+1}, \quad i = 1, \dots, \frac{n-1}{2}. \end{aligned} \tag{11}$$

The south-eastern block yields the system of the kind $\mathcal{A}_{\frac{n-1}{2}} x_{\text{even}} = b^{(1)}$ with $\mathcal{A}_{\frac{n-1}{2}} = \text{trid}_{\frac{n-1}{2}}(B^{(1)}, A^{(1)}, C^{(1)})$, where x_{even} denotes the subvector of x formed with the even block components, whose solution can be obtained by cyclically applying CR. Once the even block components of the block vector x have been computed, they can be substituted in the first part of the linear equations so that the odd block components of x are recovered. The hierarchical quasiseparability of the block matrices makes each operation of low cost.

Thus, the first (as well as the generic) step of CR performs the following steps

- (i) Given the $m \times m$ matrices A, B, C compute the matrices $A^{(1)}, B^{(1)}, C^{(1)}$.
- (ii) Given the m -vectors $b_i, i = 1, \dots, n$, compute $b_i^{(1)}, i = 1, \dots, \frac{n-1}{2}$ by means of (11).
- (iii) Recursively solve the system $\text{trid}_{\frac{n-1}{2}} x_{\text{even}} = b^{(1)}$ by means of CR.
- (iv) Compute the odd components of the solution by mean of back substitution:

$$\begin{aligned} x_1 &= A_1^{-1}(b_1 - C_1 x_2), \\ x_i &= A^{-1}(b_i - Bx_{i-1} - Cx_{i+1}), \quad i = 3, 5, \dots, n-2, \\ x_n &= A^{-1}(b_1 - Bx_{n-1}), \end{aligned}$$

In the case where the blocks A, B, C are quasiseparable, say, they are tridiagonal, not necessarily Toeplitz as in [13], and relying on the \mathcal{H} -matrix representation as in [9], in view of the preservation of the hierarchical structure of the blocks $A^{(h)}, B^{(h)}, C^{(h)}$ shown in the previous sections, the cost of step (i) is $O(m \log^2 m)$, while the costs of steps (ii) and (iv) is $O(nm \log m)$. Therefore, indicating with $T(m, n)$ the asymptotic computational complexity of the whole algorithm with $n = 2^k - 1$, we have

$$T(m, n) = T\left(m, \frac{n-1}{2}\right) + O(m \log^2 m) + O(nm \log m).$$

Since $T(m, 1) = O(m \log^2 m)$, we obtain $T(m, n) = O(mn \log m) + O(m \log^2 m \log n)$. For $m = n$ this yields $T(n, n) = O(n^2 \log n) + O(n \log^3 n)$.

It is interesting to recall that if \mathcal{A}_n is the discrete Laplacian where $A = \text{trid}_n(-1, 4, -1)$, $B = C = -I$ then CR has a cost of $O(n^2 \log n)$ ops [26] while the fast Poisson solvers based on the combination of Fourier analysis and CR [16] have a cost of $O(n^2 \log \log n)$ ops. Our approach has a slightly higher cost but covers a wider range of cases including block tridiagonal block Toeplitz matrices with banded (not necessarily Toeplitz) blocks.

Observe that CR preserves slightly more general structures than the block tridiagonal block Toeplitz. In particular it is possible to handle the case where the first and last blocks in the main diagonal differ from the other blocks on the same diagonal [10].

6.1 Solving certain generalized Sylvester equations

For an $m \times n$ matrix X denote $x = \text{vec}(X)$ the mn -vector obtained by stacking the columns of X . Then, for any pair of matrices A, B of compatible sizes, one has $\text{vec}(AB) = (I \otimes A)\text{vec}(B) = (B^t \otimes I)\text{vec}(A)$.

Consider the linear matrix equation

$$\sum_{i=1}^s A_i X B_i = C, \quad A_i \in \mathbb{R}^{m \times m}, B_i \in \mathbb{R}^{n \times n}, X, C \in \mathbb{R}^{m \times n}, \quad (12)$$

and suppose that B_i , $i = 1, \dots, s$ are tridiagonal Toeplitz matrices.

Applying the vec operator on both sides of (12) we get the $mn \times mn$ linear system

$$Wx = c, \quad W = \sum_{i=1}^s B_i^t \otimes A_i, \quad x = \text{vec}(X), \quad c = \text{vec}(C). \quad (13)$$

Since each term $B_i^t \otimes A_i$ is block tridiagonal and block Toeplitz, then the coefficient matrix of (13) is block tridiagonal, block Toeplitz as well. If the matrices A_i are k_i -quasiseparable then the blocks of W are k -quasiseparable with $k = \sum_{i=1}^s k_i$. If k is negligible with respect to m then we may solve the generalized Sylvester equation by means of QCR.

6.2 Numerical results

A possible application of this algorithm is solving discretized partial differential equations coming from convection diffusion problems of the form

$$-\epsilon \Delta u(x, y) + \mathbf{w} \cdot \nabla u(x, y) = f(x, y), \quad \Omega \subset \mathbb{R}^2 \quad (14)$$

where $u(x, y)$ is the unknown function, and we assume that the convection vector \mathbf{w} depends only on one of the two coordinates. For simplicity we assume that it only depends on x . According to [25] we can discretize the above problem obtaining the following Sylvester equation in the matrix unknown U :

$$\epsilon T_1 U + \epsilon U T_2 + \Phi_1 B_1 U + \Phi_2 U B_2 = F.$$

The independence on y of the convection vector ensures that all the right factors in the previous equation are almost Toeplitz. The matrices Φ_i are diagonal while T_i and B_i arise from the discretization of the differential operators and they are all tridiagonal and Toeplitz with the exceptions of the first and last rows (due to the boundary conditions). The matrix F contains the evaluations of the function f on the discretized grid. We refer to [25] for an in depth analysis.

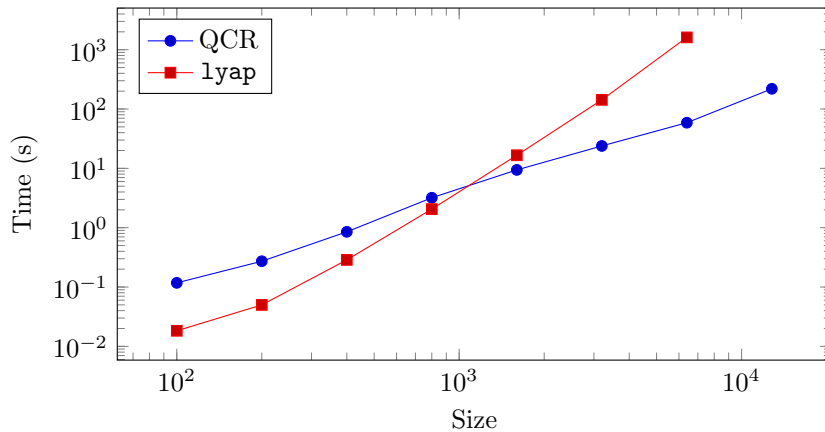


Figure 4: Timings of the quasiseparable cyclic reduction (QCR) and the Sylvester solver implemented in the `lyap` function in MATLAB.

Size	T_{QCR} (s)	Res_{QCR}	T_{lyap} (s)	Res_{lyap}
100	0.12	$2.16 \cdot 10^{-13}$	$1.83 \cdot 10^{-2}$	$1.18 \cdot 10^{-12}$
200	0.27	$1.54 \cdot 10^{-12}$	$4.99 \cdot 10^{-2}$	$5.56 \cdot 10^{-12}$
400	0.85	$5.53 \cdot 10^{-12}$	0.29	$5.17 \cdot 10^{-11}$
800	3.2	$4.19 \cdot 10^{-11}$	2.06	$9.04 \cdot 10^{-11}$
1,600	9.42	$1.25 \cdot 10^{-10}$	16.63	$5.64 \cdot 10^{-10}$
3,200	23.86	$6.78 \cdot 10^{-10}$	142.78	$2.06 \cdot 10^{-9}$
6,400	58.79	$2.41 \cdot 10^{-9}$	1,612	$2.98 \cdot 10^{-8}$
12,800	219.27	$7.8 \cdot 10^{-9}$	—	—

Table 1: Timings and residues of the Sylvester equation solved by means of the quasiseparable cyclic reduction (QCR) and the Sylvester solver implemented in the `lyap` function of MATLAB. The residues are computed by evaluating $\|\epsilon T_1 U + \epsilon U T_2 + \Phi_1 B_1 U - D\|_2$.

We performed some numerical tests on one of the example in [25] namely (14) with $\epsilon = 0.0333$ and $\mathbf{w} = (1 + \frac{(x+1)^2}{4}, 0)$. The right-hand side F is chosen at random. Since in this case $\Phi_2 = 0$ the problem is reduced to solving the Sylvester equation

$$(\epsilon T_1 + \Phi_1 B_1)U + U \epsilon T_2 = F.$$

In Figure 4 and Table 1 we compare the timings and the residue of QCR with those of the function `lyap` from the control toolbox of MATLAB R2013a. Note that our approach can be applied even if the second coordinate of \mathbf{w} is non zero and dependent only on x . In fact, in this way we retrieve a generalized Sylvester equation that can be solved with this algorithm.

7 Concluding remarks

In this work we have provided an alternative analysis, with respect to [9], of the numerical preservation of the quasiseparable structures of the matrices generated by the cyclic reduction.

The theoretical results that we have obtained better describe the phenomenon in many instances coming from the applications. Examples related to the solution of Sylvester equations arising in the discretization of elliptic PDEs, and from queuing theory, have been shown.

The connection between the numerical preservation of the structure and the existence of accurate solutions of certain discrete rational approximation problems have been pointed out.

In the second part, the use of CR, together with hierarchical representations, as a direct method for the solution of block tridiagonal “almost” Toeplitz systems has been explored and has led to the algorithm QCR. This procedure has an asymptotic complexity of $O(mn \log m) + O(m \log^2 m \log n)$, where n is the number of the blocks and m their size. Applications to the solution of elliptic differential equations have been shown and the effectiveness of the approach reported.

Applications to solving certain generalized Sylvester equations, of the form

$$\sum_{i=1}^k A_i X B_i = D,$$

have been shown in the case where all the blocks B_i s are tridiagonal Toeplitz (possibly with only the first and last row with different entries), and the A_i s have a low quasiseparable rank. Under these hypothesis, and the assumption that the sum of the quasiseparable ranks of the A_i s is negligible compared to m , the complexity of the method is $O(m^2 \log m)$.

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