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Non-unitary CMV-decomposition

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Abstract: An important decomposition for unitary matrices, the CMV-decomposition, is extended to general non-unitary matrices. This relates to short recurrence relations constructing biorthogonal bases for a particular pair of extended Krylov subspaces.

Keywords: CMV-decomposition, Krylov subspaces, matrix decomposition, oblique projection, short recurrence relation

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1 Introduction

A Krylov subspace [7] is a subspace constructed by repeatedly multiplying a given matrix $A \in \mathbb{C}^{m \times m}$ with some vector $h \in \mathbb{C}^m$, i.e., $\text{span}\{h, Ah, A^2h, \dots\}$. Extended Krylov subspaces [4] generalize this concept by allowing multiplication with the inverse of A as well in the construction of the subspace. In this manuscript short pairs of recurrence relations are derived which construct biorthogonal bases for a pair of particular extended Krylov subspaces. These subspaces are constructed by multiplication with A and its inverse alternately. Consider (possibly) distinct vectors $v, w \in \mathbb{C}^m$, then the pair of extended Krylov subspaces considered is

$$\mathcal{K}(A, v) = \text{span}\{v, Av, A^{-1}v, A^2v, A^{-2}v, \dots\}, \quad (1)$$

$$\mathcal{S}(A^H, w) = \text{span}\{w, A^{-H}w, A^Hw, A^{-2H}w, A^{2H}w, \dots\}. \quad (2)$$

We note that when $\mathcal{K}$ has a positive (negative) power of A , $\mathcal{S}$ has a negative (positive) power of A^H . The subspace used for the CMV-decomposition [2, 8] is formed in the same way. Watkins [10] showed that, for a unitary matrix and normalized $v = w$, an orthogonal basis can be constructed by a short recurrence relation. This orthogonal basis spans $\mathcal{K}(A, v)$ and $\mathcal{S}(A^H, v)$ simultaneously. He also discussed the link to orthogonal Laurent polynomials, quadrature formulas, Szegő polynomials and, Toeplitz matrices. Here the restriction to unitary matrices is dropped. Short recurrence relations are given to construct biorthogonal bases for the involved Krylov subspaces. The connection between extended Krylov subspaces and Laurent polynomials implies short recurrence relations for biorthogonal Laurent polynomials [11]. The latter is shown by making use of the moment matrix related to the pair of extended Krylov subspaces. The link to biorthogonal Szegő polynomials [1] and quadrature rules is not discussed. Section 2 derives the main result of this manuscript, a pair of short recurrence relations to construct biorthogonal bases for the pair of extended Krylov subspaces. A sparse, factored matrix representation of these recurrence relations is also given, to reveal the oblique projection of

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A onto the subspaces. Using the moment matrix the equivalent result for Laurent polynomials is derived. The section concludes with providing the link to the paper of Watkins [10] and the CMV-decomposition. Section 3 discusses the numerical properties of the proposed recurrence relations. This discussion is limited to a proof of concept. It verifies that the recurrence relations are valid. An indication of the stability of the methods is provided. A detailed study of the numerical properties of the methods is the topic of future research.

2 Short recurrence relations

Consider a nonunitary, nonsingular matrix $A \in \mathbb{C}^{m \times m}$, vectors $v, w \in \mathbb{C}^m$ and the pair of subspaces $\mathcal{K}(A, v)$ (1) and $\mathcal{S}(A^H, w)$ (2). The goal is to construct biorthogonal bases V_l and W_l for the finite extended Krylov subspaces $\mathcal{K}_l(A, v)$ and $\mathcal{S}_l(A^H, w)$, respectively. These subspaces are, for a nonnegative integer k :

For even $l = 2k$,

$$\begin{aligned}\mathcal{K}_l(A, v) &= \text{span}\{v, Av, A^{-1}v, A^2v, A^{-2}v, \dots, A^kv, A^{-k}v\}, \\ \mathcal{S}_l(A^H, w) &= \text{span}\{w, A^{-H}w, A^Hw, A^{-2H}w, A^{2H}w, \dots, A^{-kH}w, A^{kH}w\}.\end{aligned}$$

For odd $l = 2k + 1$,

$$\begin{aligned}\mathcal{K}_l(A, v) &= \text{span}\{v, Av, A^{-1}v, A^2v, A^{-2}v, \dots, A^kv, A^{-k}v, A^{k+1}v\}, \\ \mathcal{S}_l(A^H, w) &= \text{span}\{w, A^{-H}w, A^Hw, A^{-2H}w, A^{2H}w, \dots, A^{-kH}w, A^{kH}w, A^{(-k-1)H}w\}.\end{aligned}$$

The biorthogonal bases are formed by the columns of the matrices

$$V_l = \begin{bmatrix} v_0 & v_1 & v_2 & \dots & v_l \end{bmatrix}, \quad (3)$$

$$W_l = \begin{bmatrix} w_0 & w_1 & w_2 & \dots & w_l \end{bmatrix}. \quad (4)$$

The columns of these matrices, i.e., the basis vectors v_i and w_i , must satisfy the conditions

- $\text{span}\{v_0, v_1, \dots, v_l\} = \mathcal{K}_l(A, v)$,
- $\text{span}\{w_0, w_1, \dots, w_l\} = \mathcal{S}_l(A^H, w)$,
- $W_l^H V_l = I$, called the biorthogonality conditions.

The core idea in the iterative construction of nested bases for Krylov subspaces is to start from already known bases V_{l-1} and W_{l-1} for subspaces $\mathcal{K}_{l-1}(A, v)$ and $\mathcal{S}_{l-1}(A^H, w)$ and construct V_l and W_l for subspaces $\mathcal{K}_l(A, v)$ and $\mathcal{S}_l(A^H, w)$ satisfying all aforementioned conditions. The bases V_l, W_l are obtained by computing the basis vectors v_l and w_l such that $\text{span}\{V_{l-1}, v_l\} = \mathcal{K}_l(A, v)$, $\text{span}\{W_{l-1}, w_l\} = \mathcal{S}_l(A^H, w)$ and $v_l \perp \text{span}\{W_{l-1}\} = \mathcal{S}_{l-1}(A^H, w)$, $w_l \perp \text{span}\{V_{l-1}\} = \mathcal{K}_{l-1}(A, v)$. The outset of this manuscript is to compute these basis vectors efficiently by orthogonalizing with respect to a small amount of basis vectors instead of all of them. For simplicity we assume that no breakdowns occur, neither lucky nor serious. This no-breakdown assumption implies that $\langle v_l, w_l \rangle \neq 0$ and $\mathcal{K}_l(A, v) \subset \mathcal{K}_{l+1}(A, v)$, $\mathcal{S}_l(A^H, w) \subset \mathcal{S}_{l+1}(A^H, w)$, i.e., strict subsets. Note that this also implies that $l < m$. The no-breakdown assumption is not a real restriction, since the results presented here are valid up to the occurrence of a breakdown. Our analysis will use the Euclidean inner product $\langle x, y \rangle := y^H x$. Lemma 1 provides a classical identity on which the analysis relies heavily.

Lemma 1 (Inner product property). *Consider a nonsingular matrix $A \in \mathbb{C}^{m \times m}$, two vectors $x, y \in \mathbb{C}^m$ and the Euclidean inner product $\langle \cdot, \cdot \rangle$, then the following equation holds*

$$\langle x, y \rangle = \langle Ax, A^{-H}y \rangle.$$

In numerical methods it is of interest to obtain the projection of the given matrix A onto the subspaces. Such projections should be of smaller size than A and capture as much of the relevant information present in

A as possible, e.g., model order reduction [5] and approximation of matrix functions [4] rely on this concept. These projections are given by the matrix of recurrence coefficients and exhibit a particular structure. The discussion here is restricted to projection of A onto $\mathcal{K}(A, v)$ and orthogonal to $\mathcal{S}(A^H, w)$. Its dual, projection onto $\mathcal{S}(A^H, w)$ and orthogonal to $\mathcal{K}(A, v)$, will turn out to be similar and is therefore omitted.

2.1 Four-term recurrence relation

A short (four-term) recurrence relation is derived for the biorthogonal bases V_l (3) and W_l (4). This derivation extends the results of Watkins [10], in the sense that it is not restricted to the case where A is a unitary matrix. Lemma 1 and the orthogonality properties of V_l and W_l are the key to obtain the short recurrence relations in Theorem 1.

Theorem 1. *Let $A \in \mathbb{C}^{m \times m}$ be a nonsingular matrix and $v, w \in \mathbb{C}^m$, then biorthogonal bases $V_l \in \mathbb{C}^{m \times (l+1)}$ (3) and $W_l \in \mathbb{C}^{m \times (l+1)}$ (4) can be constructed by four-term recurrence relations.*

For $l = 2k + 1$, $k \geq 0$, with $v_{-1} = v_0$, $v_{-2} = 0$ and $\alpha_{-1,0} = 0$,

$$\eta_{2k+1,2k} v_{2k+1} = A v_{2k-1} - \alpha_{2k-2,2k} v_{2k-2} - \alpha_{2k-1,2k} v_{2k-1} - \alpha_{2k,2k} v_{2k}, \quad (5)$$

$$v_{2k+1,2k} w_{2k+1} = A^H w_{2k-1} - \beta_{2k-2,2k} w_{2k-2} - \beta_{2k-1,2k} w_{2k-1} - \beta_{2k,2k} w_{2k}, \quad (6)$$

where $\alpha_{i,2k} = \langle A v_{2k-1}, w_i \rangle$ and $\beta_{i,2k} = \langle A^H w_{2k-1}, v_i \rangle$.

For $l = 2k + 2$, $k \geq 0$, with $v_{-1} = 0$,

$$\eta_{2k+2,2k+1} v_{2k+2} = A^{-1} v_{2k} - \alpha_{2k-1,2k+1} v_{2k-1} - \alpha_{2k,2k+1} v_{2k} - \alpha_{2k+1,2k+1} v_{2k+1}, \quad (7)$$

$$v_{2k+2,2k+1} w_{2k+2} = A^H w_{2k} - \beta_{2k-1,2k+1} w_{2k-1} - \beta_{2k,2k+1} w_{2k} - \beta_{2k+1,2k+2} w_{2k+1}, \quad (8)$$

where $\alpha_{i,2k+1} = \langle A^{-1} v_{2k}, w_i \rangle$ and $\beta_{i,2k+1} = \langle A^H w_{2k}, v_i \rangle$. Normalization is done by choosing $\eta_{l,l-1}$ and $v_{l,l-1}$ such that $\langle v_l, w_l \rangle = 1$. This is assumed to always be possible, i.e., the assumption that breakdowns do not occur.

Proof. Recurrence relations (5) and (7) are proven. The proof of (6) and (8) is analogous. Assume, without loss of generality, that $l = 2k$. The next basis vector v_{2k+1} must be constructed such that it expands $\mathcal{K}_{2k}(A, v)$ to $\mathcal{K}_{2k+1}(A, v)$, i.e., introduces a component along the direction $A^{k+1}v$. And it must be orthogonal to $\mathcal{S}_{2k}(A^H, w)$. Consider v_{2k-1} , with properties

$$\begin{aligned} v_{2k-1} &\in \text{span}\{v, Av, A^{-1}v, A^2v, A^{-2}v, \dots, A^{k-1}v, A^{-k+1}v, A^k v\} = \mathcal{K}_{2k-1}(A, v) \\ &\perp \text{span}\{w, A^{-H}w, A^H w, A^{-2H}w, A^{2H}w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w\} = \mathcal{S}_{2k-2}(A^H, w). \end{aligned}$$

Multiplication with A results in

$$A v_{2k-1} \in \text{span}\{Av, A^2v, v, A^3v, A^{-1}v, \dots, A^k v, A^{-k+2}v, A^{k+1}v\},$$

which shows that $A v_{2k-1}$ has a component along the required direction $A^{k+1}v$. And by the no-breakdown assumption, this vector will be linearly independent of $\mathcal{K}_{2k}(A, v)$.

Using Lemma 1, i.e., $\langle x, y \rangle = \langle Ax, A^{-H}y \rangle$, we obtain

$$\begin{aligned} A v_{2k-1} &\perp A^{-H} \text{span}\{w, A^{-H}w, A^H w, A^{-2H}w, A^{2H}w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w\} \\ &\perp \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(k-2)H}w, A^{(-k+1)H}w, A^{-kH}w\}. \end{aligned}$$

Hence, vector $A v_{2k-1}$ is orthogonal with respect to $\mathcal{S}_{2k-3}(A^H, w)$. It remains to orthogonalize it with respect to w_{2k-2} , w_{2k-1} and w_{2k} in order to satisfy the orthogonality condition $v_{2k+1} \perp \mathcal{S}_{2k}(A^H, w)$. Thus, (5) is proven, since $\alpha_{i,2k}$ is chosen such that it eliminates the aforementioned directions from $A v_{2k-1}$. Similar reasoning can be applied to construct v_{2k+2} . Consider v_{2k} , with properties

$$\begin{aligned} v_{2k} &\in \text{span}\{v, Av, A^{-1}v, \dots, A^{k-1}v, A^{-k+1}v, A^k v, A^{-k}v\} \\ &\perp \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w, A^{-kH}w\}. \end{aligned}$$

Multiplication with A^{-1} and Lemma 1, i.e., $\langle x, y \rangle = \langle A^{-1}x, A^H y \rangle$ provides

$$\begin{aligned} A^{-1}v_{2k} &\in \text{span}\{A^{-1}v, v, A^{-2}v, \dots, A^{k-2}v, A^{-k}v, A^{k-1}v, A^{-k-1}v\} \\ &\perp \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w, A^{-kH}w\}. \end{aligned}$$

Variables $\alpha_{i,2k+1}$ are chosen such that they eliminate the directions such that $v_{2k+2} \perp \mathcal{S}_{2k+1}(A^H, w)$. Thus proving (7). $\square$

Next, in Theorem 2, the matrix of recurrence coefficients is given, which has pentadiagonal structure. The projection of A onto $\mathcal{K}_l(A, h)$ and orthogonal to $\mathcal{S}_l(A^H, w)$ is given by $W_l^H A V_l = Z_l$. The projection matrix $Z_l \in \mathbb{C}^{(l+1) \times (l+1)}$ is the matrix of recurrence coefficients $\hat{Z}_l \in \mathbb{C}^{(l+2) \times (l+1)}$ with its last row removed.

Theorem 2. Consider a nonsingular matrix $A \in \mathbb{C}^{m \times m}$, $v \in \mathbb{C}^m$ and basis $V_l \in \mathbb{C}^{m \times (l+1)}$ (3) spanning $\mathcal{K}_l(A, v)$. The matrix of recurrence coefficients $\hat{Z}_l \in \mathbb{C}^{(l+2) \times (l+1)}$ satisfying

$$A V_l = V_{l+1} \hat{Z}_l,$$

has pentadiagonal structure. More precisely, for $h_{i,2k} = \langle A v_{2k}, w_i \rangle$ and, $\alpha_{i,2k} = \langle A v_{2k-1}, w_i \rangle$ and $\eta_{2k+1,2k}$ as a normalizing constant, i.e., as in Theorem 1, the matrix is

$$\hat{Z}_l = \begin{bmatrix} h_{0,0} & \alpha_{0,2} & h_{0,2} & & & \\ h_{1,0} & \alpha_{1,2} & h_{1,2} & & & \\ & \alpha_{2,2} & h_{2,2} & \alpha_{2,4} & h_{2,4} & \\ & \eta_{3,2} & h_{3,2} & \alpha_{3,4} & h_{3,4} & \\ & & & \alpha_{4,4} & h_{4,4} & \\ & & & \eta_{5,4} & h_{5,4} & \\ & & & & & \ddots \end{bmatrix}. \quad (9)$$

Proof. Consider the recurrence relation following immediately from Equation (5),

$$A v_{2k-1} = \alpha_{2k-2,2k} v_{2k-2} + \alpha_{2k-1,2k} v_{2k-1} + \alpha_{2k,2k} v_{2k} + \eta_{2k+1,2k} v_{2k+1}.$$

This relation forms the even columns of $\hat{Z}_l$. To obtain a recurrence relation for $A v_{2k}$, i.e., the odd columns of $\hat{Z}_l$, look at the space in which this vector lives

$$\begin{aligned} v_{2k} &\in \text{span}\{v, A v, A^{-1}v, \dots, A^k v, A^{-k}v\} \\ A v_{2k} &\in \text{span}\{A v, A^2 v, v, \dots, A^k v, A^{-k+2}v, A^{k+1}v, A^{-k+1}v\} \\ &\subseteq \text{span}\{v, A v, A^{-1}v, \dots, A^{-k+1}v, A^k v, A^{-k}v, A^{k+1}v\} \\ &= \text{span}\{v_0, \dots, v_{2k}, v_{2k+1}\}. \end{aligned}$$

Hence, $A v_{2k} = \sum_{i=0}^{2k+1} h_{i,2k} v_i$. A short recurrence relation is obtained by looking at orthogonality properties

$$\begin{aligned} v_{2k} &\perp \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w, A^{-kH}w\} \\ A v_{2k} &\perp A^{-H} \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(-k+1)H}w, A^{(k-1)H}w, A^{-kH}w\} \\ &\perp \text{span}\{w, A^{-H}w, A^H w, \dots, A^{(k-2)H}w, A^{(-k+1)H}w, A^{-kH}w, A^{(-k-1)H}w\} \\ &\perp \text{span}\{w_0, \dots, w_{2k-4}, w_{2k-3}\}. \end{aligned}$$

Thus the short recurrence relation, with $h_{i,2k} = \langle A v_{2k}, w_i \rangle$, is

$$A v_{2k} = h_{2k-2,2k} v_{2k-2} + h_{2k-1,2k} v_{2k-1} + h_{2k,2k} v_{2k} + h_{2k+1,2k} v_{2k+1}.$$

$\square$

The four term recurrence relation contains some redundant information. This is suggested by the similarity of the coefficients $\alpha_{i,l}$ and $\beta_{i,l}$ occurring in Theorem 1 and verified by the low rank structure appearing in the matrix of recurrence coefficients $\hat{Z}_l$. Example 1 illustrates the low rank structure of $\hat{Z}_l$.

Example 1. Following the notation of Theorem 2, let $l = 6$. Then the matrix of recurrence coefficients

$$\hat{Z}_6 = \begin{bmatrix} \times & \times & * & & & \\ \times & \times & * & & & \\ & * & \times & \times & * & \\ & * & \times & \times & * & \\ & & & * & \times & \times & * \\ & & & * & \times & \times & * \\ & & & & & * & \times \\ & & & & & & * & \times \end{bmatrix},$$

where $\times$ and $*$ denote a generic nonzero element, exhibits some low rank structure. Namely, the pairs of nonzero elements represented as $*$ equal their neighbouring elements $\times$ multiplied with the same factor. Or in other words, every submatrix

$$\begin{bmatrix} \times & * \\ \times & * \end{bmatrix} \text{ or } \begin{bmatrix} * & \times \\ * & \times \end{bmatrix}$$

has rank equal to 1. This implies that there is redundant information present in $\hat{Z}_l$.

2.2 Two-term recurrence relation

The low rank structure in the matrix of recurrence coefficients $\hat{Z}_l$ from Theorem 2 implies that a shorter (2-term) recurrence relation can be derived for the bases V_l and W_l , respectively spanning the $(l+1)$ -dimensional subspaces of

$$\begin{aligned} \mathcal{K}(A, v) &= \text{span}\{v, Av, A^{-1}v, A^2v, A^{-2}v, \dots\}, \\ \mathcal{S}(A^H, w) &= \text{span}\{w, A^{-H}w, A^Hw, A^{-2H}w, A^{2H}w, \dots\}. \end{aligned}$$

As before, they satisfy the conditions

- $\text{span}\{v_0, v_1, \dots, v_l\} = \mathcal{K}_l(A, v)$,
- $\text{span}\{w_0, w_1, \dots, w_l\} = \mathcal{S}_l(A^H, w)$,
- $W_l^H V_l = I$.

The shorter recurrence relation is achieved by simultaneously building biorthogonal bases for

$$\begin{aligned} \mathcal{S}(A, v) &= \text{span}\{v, A^{-1}v, Av, A^{-2}v, A^2v, \dots\}, \\ \mathcal{K}(A^H, w) &= \text{span}\{w, A^Hw, A^{-H}w, A^{2H}w, A^{-2H}w, \dots\}. \end{aligned}$$

Thus we have now 4 subspaces: $\mathcal{K}(A, v)$, $\mathcal{S}(A, v)$, $\mathcal{K}(A^H, w)$, $\mathcal{S}(A^H, w)$. Consider the matrices

$$\tilde{V}_l = \begin{bmatrix} \tilde{v}_0 & \tilde{v}_1 & \tilde{v}_2 & \dots & \tilde{v}_l \end{bmatrix}, \quad (10)$$

$$\tilde{W}_l = \begin{bmatrix} \tilde{w}_0 & \tilde{w}_1 & \tilde{w}_2 & \dots & \tilde{w}_l \end{bmatrix}, \quad (11)$$

whose columns satisfy the conditions

- $\text{span}\{\tilde{v}_0, \tilde{v}_1, \dots, \tilde{v}_l\} = \mathcal{S}_l(A, v)$,
- $\text{span}\{\tilde{w}_0, \tilde{w}_1, \dots, \tilde{w}_l\} = \mathcal{K}_l(A^H, w)$,

$$- \tilde{W}_l^H \tilde{V}_l = I.$$

The recurrence relations are given in Theorem 3.

Theorem 3. Let $A \in \mathbb{C}^{m \times m}$ be a nonsingular matrix and $v, w \in \mathbb{C}^m$, then biorthogonal bases V_l (3), W_l (4), $\tilde{V}_l$ (10) and $\tilde{W}_l$ (11) can be constructed by pairs of two-term recurrence relations.

For $l = 2k + 1$, $k \geq 0$,

$$\eta_{2k} v_{2k+1} = A \tilde{v}_{2k} - \gamma_{2k} v_{2k}, \quad (12)$$

$$\tilde{\eta}_{2k} \tilde{v}_{2k+1} = A^{-1} v_{2k} - \tilde{\gamma}_{2k} \tilde{v}_{2k}, \quad (13)$$

$$v_{2k} w_{2k+1} = A^{-H} \tilde{w}_{2k} - \tilde{\gamma}_{2k} w_{2k}, \quad (14)$$

$$\tilde{v}_{2k} \tilde{w}_{2k+1} = A^H w_{2k} - \tilde{\gamma}_{2k} \tilde{w}_{2k}, \quad (15)$$

where $\gamma_{2k} = \langle A \tilde{v}_{2k}, w_{2k} \rangle$ and $\tilde{\gamma}_{2k} = \langle A^{-1} v_{2k}, \tilde{w}_{2k} \rangle$.

For $l = 2k + 2$, $k \geq 0$,

$$\eta_{2k+1} v_{2k+2} = \tilde{v}_{2k+1} - \gamma_{2k+1} v_{2k+1}, \quad (16)$$

$$\tilde{\eta}_{2k+1} \tilde{v}_{2k+2} = v_{2k+1} - \tilde{\gamma}_{2k+1} \tilde{v}_{2k+1}, \quad (17)$$

$$v_{2k+1} w_{2k+2} = \tilde{w}_{2k+1} - \tilde{\gamma}_{2k+1} w_{2k+1}, \quad (18)$$

$$\tilde{v}_{2k+1} \tilde{w}_{2k+2} = w_{2k+1} - \tilde{\gamma}_{2k+1} \tilde{w}_{2k+1}, \quad (19)$$

where $\gamma_{2k+1} = \langle \tilde{v}_{2k+1}, w_{2k+1} \rangle$ and $\tilde{\gamma}_{2k+1} = \langle v_{2k+1}, \tilde{w}_{2k+1} \rangle$. Normalization coefficients $\eta_i, v_i, \tilde{\eta}_i$ and $\tilde{v}_i$ are chosen such that $\langle v_i, w_i \rangle = 1$ and $\langle \tilde{v}_i, \tilde{w}_i \rangle = 1$. This is assumed to be possible under the no-breakdown assumption.

Proof. The proof is given here for (12), (13), (16) and (17). For the remaining recurrence relations the proof is analogous. Assume, without loss of generality, $l = 2k$. The next basis vector v_{2k+1} must be constructed such that it expands $\mathcal{K}_{2k}(A, v)$ to $\mathcal{K}_{2k+1}(A, v)$, i.e., introduce a component along the direction $A^{k+1}v$. And it must be orthogonal to $\mathcal{S}_{2k}(A^H, w)$. Consider

$$\begin{aligned} \tilde{v}_{2k} &\in \text{span}\{v, A^{-1}v, Av, \dots, A^{-k}v, A^k v\} = \mathcal{S}_{2k}(A, v) \\ &\perp \text{span}\{w, A^H w, A^{-H} w, \dots, A^{(-k+1)H} w, A^{kH} w\} = \mathcal{K}_{2k-1}(A^H, w). \end{aligned}$$

Multiplication with A and Lemma 1 provides us with

$$A \tilde{v}_{2k} \in \text{span}\{Av, v, A^2 v, \dots, A^{-k+1} v, A^{k+1} v\} \quad (20)$$

$$\begin{aligned} &\perp A^{-H} \text{span}\{w, A^H w, A^{-H} w, \dots, A^{(-k+1)H} w, A^{kH} w\} \\ &\perp \text{span}\{w, A^H w, A^{-H} w, \dots, A^{(k-1)H} w, A^{-kH} w\} = \mathcal{S}_{2k-1}(A^H, w). \end{aligned} \quad (21)$$

The required component $A^{k+1}v$ is present (20) and orthogonality is satisfied with respect to $\mathcal{S}_{2k-1}(A^H, w)$ (21). Note that $A \tilde{v}_{2k}$ is orthogonal to a larger subspace of $\mathcal{S}_{2k}(A^H, w)$ than Av_{2k-1} , this is the key observation to explain the shorter recurrence relation. Orthogonalization only remains to be done to eliminate components along w_{2k} , thus obtaining (12). The same derivation can be done for $\tilde{v}_{2k+1}$, which must expand $\mathcal{S}_{2k}(A, v)$ to $\mathcal{S}_{2k+1}(A, v)$ and must be orthogonal to $\mathcal{K}_{2k}(A^H, w)$. Thereby proving (13). For v_{2k+2} , consider $\tilde{v}_{2k+1}$

$$\tilde{v}_{2k+1} \in \text{span}\{v, A^{-1}v, Av, \dots, A^{-k}v, A^k v, A^{-k-1} v\} \quad (22)$$

$$\perp \text{span}\{w, A^H w, A^{-H} w, \dots, A^{kH} w, A^{-kH} w\} = \mathcal{S}_{2k}(A^H, w). \quad (23)$$

The component along $A^{-k-1}v$ is present in $\tilde{v}_{2k+1}$ (22). So it only remains to enforce the orthogonality conditions, orthogonalize along w_{2k+1} to obtain (16). Similarly for $\tilde{v}_{2k+2}$, to obtain (17). $\square$

From these recurrence relations, a matrix pencil representation of the matrix of recurrence coefficients $\hat{Z}_l$ from Theorem 2 can be derived. This result is given in Theorem 4. This representation reveals that $\hat{Z}_l$ can be represented by a product of essentially 2×2 matrices. This allows for an efficient way to store and manipulate this matrix on a computer.

Theorem 4. Consider a nonsingular matrix $A \in \mathbb{C}^{m \times m}$, $v, w \in \mathbb{C}^m$ and basis $V_l \in \mathbb{C}^{m \times (l+1)}$ (3) spanning $\mathcal{K}_l(A, v)$. The matrix pencil of recurrence coefficients $(\hat{T}_l, \hat{S}_l)$, with $\hat{T}_l, \hat{S}_l \in \mathbb{C}^{(l+2) \times (l+1)}$ satisfying

$$AV_{l+1}\hat{S}_l = V_{l+1}\hat{T}_l,$$

can be represented by two tridiagonal matrices with a particular structure. More precisely, for the same coefficients as used in Theorem 3,

$$\hat{T}_l = \begin{bmatrix} \gamma_0 & \tilde{\eta}_0^{-1}(1 - \gamma_0\tilde{\gamma}_0) & & & \\ \eta_0 & -\tilde{\eta}_0^{-1}\eta_0\tilde{\gamma}_0 & & & \\ & & \gamma_2 & \tilde{\eta}_2^{-1}(1 - \gamma_2\tilde{\gamma}_2) & \\ & & \eta_2 & -\tilde{\eta}_2^{-1}\eta_2\tilde{\gamma}_2 & \\ & & & & \gamma_4 \\ & & & & \eta_4 \\ & & & & & \ddots \end{bmatrix}$$

$$\hat{S}_l = \begin{bmatrix} 1 & & & & \\ \gamma_1 & \tilde{\eta}_1^{-1}(1 - \gamma_1\tilde{\gamma}_1) & & & \\ \eta_1 & -\tilde{\eta}_1^{-1}\eta_1\tilde{\gamma}_1 & & & \\ & & \gamma_3 & \tilde{\eta}_3^{-1}(1 - \gamma_3\tilde{\gamma}_3) & \\ & & \eta_3 & -\tilde{\eta}_3^{-1}\eta_3\tilde{\gamma}_3 & \\ & & & & \ddots \end{bmatrix}.$$

Proof. Rewrite the pairs of recurrence relations (12), (13), (16) and (17) in matrix notation to obtain

$$A \begin{bmatrix} \tilde{v}_{2k} & \tilde{v}_{2k+1} \end{bmatrix} = \begin{bmatrix} v_{2k} & v_{2k+1} \end{bmatrix} \begin{bmatrix} \gamma_{2k} & \tilde{\eta}_{2k}^{-1}(1 - \gamma_{2k}\tilde{\gamma}_{2k}) \\ \eta_{2k} & -\tilde{\eta}_{2k}^{-1}\eta_{2k}\tilde{\gamma}_{2k} \end{bmatrix}, \quad (24)$$

$$\begin{bmatrix} \tilde{v}_{2k+1} & \tilde{v}_{2k+2} \end{bmatrix} = \begin{bmatrix} v_{2k+1} & v_{2k+2} \end{bmatrix} \begin{bmatrix} \gamma_{2k+1} & \tilde{\eta}_{2k+1}^{-1}(1 - \gamma_{2k+1}\tilde{\gamma}_{2k+1}) \\ \eta_{2k+1} & -\tilde{\eta}_{2k+1}^{-1}\eta_{2k+1}\tilde{\gamma}_{2k+1} \end{bmatrix}. \quad (25)$$

The proof consists of substituting (25) into (24). Substitution is done as follows, consider

$$A \begin{bmatrix} \tilde{v}_{2k} & \tilde{v}_{2k+1} & \tilde{v}_{2k+2} & \tilde{v}_{2k+3} \end{bmatrix} = \begin{bmatrix} v_{2k} & v_{2k+1} & v_{2k+2} & v_{2k+3} \end{bmatrix} \begin{bmatrix} D_{2k} & \\ & D_{2k+2} \end{bmatrix},$$

where $D_i = \begin{bmatrix} \gamma_i & \tilde{\eta}_i^{-1}(1 - \gamma_i\tilde{\gamma}_i) \\ \eta_i & -\tilde{\eta}_i^{-1}\eta_i\tilde{\gamma}_i \end{bmatrix}$. Then (24) can be used to obtain

$$A \begin{bmatrix} \tilde{v}_{2k} & v_{2k+1} & v_{2k+2} & \tilde{v}_{2k+3} \end{bmatrix} \begin{bmatrix} 1 & & & \\ & D_{2k+1} & & \\ & & 1 & \\ & & & 1 \end{bmatrix} = \begin{bmatrix} v_{2k} & v_{2k+1} & v_{2k+2} & v_{2k+3} \end{bmatrix} \begin{bmatrix} D_{2k} & & & \\ & D_{2k+2} & & \end{bmatrix}.$$

Repeating this procedure for $v_i, \tilde{v}_i, i = 0, 1, \dots, l$ proves the statement. $\square$

Note that the structures of the matrices of recurrence coefficients appearing in Theorem 2 and Theorem 4 are known [9]. The contribution of this manuscript is the procedure to compute these matrices in an efficient manner.

2.3 Levinson type derivation

The two-term recurrence relation can also be derived starting from the moment matrix arising from the subspaces $\mathcal{K}(A, v)$ and $\mathcal{S}(A^H, w)$. The derivation here will follow a Levinson type procedure. Such procedures

rely on the isomorphism between a vector space of $(n+1)$ -tuples and of polynomials of degree n . In the case studied here, the connection between vectors $v_n \in \mathcal{K}_n(A, v)$ and Laurent polynomials $a_n \in \mathcal{F}_n(z)$ is used. Similar to the definition of $\mathcal{K}_l(A, v)$ and $\mathcal{S}_l(A^H, w)$, we define, for a nonnegative integer k :

For even $l = 2k$,

$$\begin{aligned}\mathcal{F}_l(z) &= \text{span}\{1, z, z^{-1}, z^2, z^{-2}, \dots, z^k, z^{-k}\}, \\ \mathcal{S}_l(z) &= \text{span}\{1, z^{-1}, z, z^{-2}, z^2, \dots, z^{-k}, z^k\}.\end{aligned}$$

For odd $l = 2k + 1$,

$$\begin{aligned}\mathcal{F}_l(z) &= \text{span}\{1, z, z^{-1}, z^2, z^{-2}, \dots, z^k, z^{-k}, z^{k+1}\}, \\ \mathcal{S}_l(z) &= \text{span}\{1, z^{-1}, z, z^{-2}, z^2, \dots, z^{-k}, z^k, z^{-k-1}\}.\end{aligned}$$

Because $v_n \in \mathcal{K}_n(A, v)$, we can write v_n in terms of a corresponding Laurent polynomial $a_n(z) \in \mathcal{F}_n(z)$, i.e., $v_n = a_n(A)v$. Similarly, $w_n = b_n(A^H)w$. Consider the bases, i.e., columns representing the basis vectors,

$$\begin{aligned}K &= \begin{bmatrix} v & Av & A^{-1}v & A^2v & A^{-2}v & \dots \end{bmatrix}, \\ S &= \begin{bmatrix} w & A^{-H}w & A^Hw & A^{-2H}w & A^{2H}w & \dots \end{bmatrix}\end{aligned}$$

for $\mathcal{K}(A, v)$ and $\mathcal{S}(A^H, w)$, respectively.

Then the corresponding moment matrix M , with $m_i := w^H A^i v = \langle A^i v, w \rangle$, is

$$\begin{aligned}M &= S^H K \\ &= \begin{bmatrix} m_0 & m_1 & m_{-1} & m_2 & m_{-2} & & \\ m_{-1} & m_0 & m_{-2} & m_1 & m_{-3} & & \\ m_1 & m_2 & m_0 & m_3 & m_{-1} & \dots & \\ m_{-2} & m_{-1} & m_{-3} & m_0 & m_{-4} & & \\ m_2 & m_3 & m_1 & m_4 & m_0 & & \\ & & \vdots & & & \ddots & \end{bmatrix}. \end{aligned} \quad (26)$$

Note that $\tilde{M} = \tilde{S}^H \tilde{K} = M^\top$, where

$$\tilde{K} = \begin{bmatrix} v & A^{-1}v & Av & A^{-2}v & A^2v & \dots \end{bmatrix}$$

is a basis for $\mathcal{S}(A, v)$ and

$$\tilde{S} = \begin{bmatrix} w & A^{-H}w & A^Hw & A^{-2H}w & A^{2H}w & \dots \end{bmatrix}$$

a basis for $\mathcal{K}(A^H, w)$. The highly structured nature of M suggests short recurrence relations. Remark that a certain permutation of the rows and columns of M results in a block matrix, where the two diagonal blocks are Hankel and the two off-diagonal blocks are Toeplitz matrices. This reveals the low displacement rank [6] of the moment matrix. To derive the recurrence relations, we require three more matrices. A matrix P which allows, by multiplication from the left, to represent a vector in $\{1, z^{-1}, z, z^{-2}, z^2, \dots\}$ in the basis $\{1, z, z^{-1}, z^2, z^{-2}, \dots\}$ and vice versa. A matrix Z representing multiplication with z in basis $\{1, z, z^{-1}, z^2, z^{-2}, \dots\}$ and $\tilde{Z}$ representing multiplication with z^{-1} in basis $\{1, z^{-1}, z, z^{-2}, z^2, \dots\}$. Matrix P is a permutation matrix,

$$P = \begin{bmatrix} 1 & & & & & \\ & 0 & 1 & & & \\ & 1 & 0 & & & \\ & & & 0 & 1 & \\ & & & 1 & 0 & \\ & & & & & \ddots \end{bmatrix}$$

and the matrices representing multiplication with z and z^{-1} , respectively are

$$Z = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ & & & & & \ddots \end{bmatrix}, \quad \tilde{Z} = Z^\top.$$

An important observation is that, for $Z_{2k} \in \mathbb{C}^{(2k+1) \times (2k+1)}$, the $(2k+1) \times (2k+1)$ principal submatrix of Z and $e_{2k} \in \mathbb{C}^{2k+1}$ the $2k$ th column of the unit matrix,

$$z \begin{bmatrix} 1 & z^1 & z^{-1} & z^2 & z^{-2} & \dots & z^k & z^{-k} \end{bmatrix} = \begin{bmatrix} 1 & z^1 & z^{-1} & z^2 & z^{-2} & \dots & z^k & z^{-k} \end{bmatrix} Z_{2k} + z^{k+1} e_{2k}^\top.$$

So Z_{2k} represents multiplication with z in the basis $\{1, z, z^{-1}, z^2, z^{-2}, \dots, z^k, z^{-k}\}$ up to a rank one term. Before providing the two term recurrence relations in terms of Laurent polynomials in Theorem 5, an appropriate inner product must be defined.

Definition 1 (Inner product for Laurent polynomials). *Let $A \in \mathbb{C}^{m \times m}$, $v, w \in \mathbb{C}^m$ and $l(z), \hat{l}(z)$ be two Laurent polynomials. Then the inner product is*

$$\langle l(z), \hat{l}(z) \rangle := w^H \tilde{l}(A) l(A) v, \quad (27)$$

where $\tilde{l}(z)$ denotes the same Laurent polynomial as $\hat{l}(z)$ with its coefficients complex conjugated.

The inner product in Definition 1 relates closely to the Euclidean product from above.

Theorem 5. *Consider the Laurent polynomials $a_i(z), \tilde{b}_i(z) \in \mathcal{F}_i(z)$ and $\tilde{a}_i(z), b_i(z) \in \mathcal{G}_i(z)$. If they are constructed via*

$$\begin{aligned} \eta_{2k} a_{2k+1}(z) &= z \tilde{a}_{2k}(z) - \gamma_{2k} a_{2k}(z), \\ \tilde{\eta}_{2k} \tilde{a}_{2k+1}(z) &= z^{-1} a_{2k}(z) - \tilde{\gamma}_{2k} \tilde{a}_{2k}(z), \\ \nu_{2k} b_{2k+1}(z) &= z^{-1} \tilde{b}_{2k}(z) - \tilde{\gamma}_{2k} b_{2k}(z), \\ \tilde{\nu}_{2k} \tilde{b}_{2k+1}(z) &= z b_{2k}(z) - \tilde{\gamma}_{2k} \tilde{b}_{2k}(z), \\ \eta_{2k+1} a_{2k+2}(z) &= \tilde{a}_{2k+1}(z) - \gamma_{2k+1} a_{2k+1}(z), \\ \tilde{\eta}_{2k+1} \tilde{a}_{2k+2}(z) &= a_{2k+1}(z) - \tilde{\gamma}_{2k+1} \tilde{a}_{2k+1}(z), \\ \nu_{2k+1} b_{2k+2}(z) &= \tilde{b}_{2k+1}(z) - \tilde{\gamma}_{2k+1} b_{2k+1}(z), \\ \tilde{\nu}_{2k+1} \tilde{b}_{2k+2}(z) &= b_{2k+1}(z) - \tilde{\gamma}_{2k+1} \tilde{b}_{2k+1}(z), \end{aligned}$$

where $\gamma_{2k} = \langle z \tilde{a}_{2k}, b_{2k} \rangle$, $\tilde{\gamma}_{2k} = \langle z^{-1} a_{2k}, \tilde{b}_{2k} \rangle$, $\gamma_{2k+1} = \langle \tilde{a}_{2k+1}, b_{2k+1} \rangle$ and $\tilde{\gamma}_{2k+1} = \langle a_{2k+1}, \tilde{b}_{2k+1} \rangle$. Then the sequences $\{a_i(z)\}_i$ and $\{b_i(z)\}_i$ form biorthogonal Laurent polynomials. That is, if η_i, ν_i are chosen such that $\langle a_i(z), b_i(z) \rangle = 1$, then $\langle a_i(z), b_j(z) \rangle = \delta_{ij}$, biorthogonal with respect to the inner product from Definition 1. Similarly for $\{\tilde{a}_i(z)\}_i$ and $\{\tilde{b}_i(z)\}_i$.

Proof. The proof is given by induction and follows a Levinson-type derivation. Consider the moment matrix $M_0 := \begin{bmatrix} m_0 \end{bmatrix}$, then $a_0 := m_0^{-1/2}$ and $b_0 := \overline{m_0}^{-1/2}$ satisfy the biorthonormality condition $\langle a_0, b_0 \rangle = 1$. Assume, without loss of generality, that $n = 2k$ and $a_n(z), \tilde{a}_n(z)$ are such that their coefficients $a_n, \tilde{a}_n \in \mathbb{C}^{n+1}$ with

respect to bases $\{1, z, z^{-1}, z^2, z^{-2}, \dots, z^k, z^{-k}\}$ and $\{1, z^{-1}, z, z^{-2}, z^2, \dots, z^{-k}, z^k\}$, respectively, satisfy

$$M_n \begin{bmatrix} a_n \end{bmatrix} = \begin{bmatrix} m_0 & m_1 & m_{-1} & \dots & m_k & m_{-k} \\ m_{-1} & m_0 & m_{-2} & \dots & m_{k-1} & m_{-k-1} \\ m_1 & m_2 & m_0 & \dots & m_{k+1} & m_{-k+1} \\ \vdots & & & \ddots & & \vdots \\ m_{-k} & m_{-k+1} & m_{-k-1} & \dots & m_0 & m_{-2k} \\ m_k & m_{k+1} & m_{k-1} & \dots & m_{2k} & m_0 \end{bmatrix} \begin{bmatrix} a_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \tau_n \end{bmatrix}$$

and

$$\tilde{M}_n \begin{bmatrix} \tilde{a}_n \end{bmatrix} = M_n^\top \begin{bmatrix} \tilde{a}_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \tilde{\tau}_n \end{bmatrix}.$$

These are matrix representations of orthogonality conditions [3, p.44]. Orthogonality is interpreted as follows, vector a_n in the basis formed by the columns of K_n , i.e., $K_n a_n$, is orthogonal to the space spanned by the columns of S_{n-1} , i.e., $S_{n-1}^H K_n a_n = 0$. Then, for the next moment matrix M_{n+1} and $\begin{bmatrix} a_n & 0 \end{bmatrix}^\top$, the embedding of $a_n \in \mathbb{C}^{n+1}$ in the space $\mathbb{C}^{n+2}$, further denoted simply by a_n (same for $\tilde{a}_n$), we obtain

$$M_{n+1} \begin{bmatrix} a_n \end{bmatrix} = \begin{bmatrix} & & & m_{k+1} \\ & M_n & & m_k \\ & & & \vdots \\ m_{-k-1} & m_{-k} & \dots & m_0 \end{bmatrix} \begin{bmatrix} a_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tau_n \end{bmatrix} \quad \text{and} \quad M_{n+1} Z_{n+1} P_{n+1} \begin{bmatrix} \tilde{a}_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{\alpha}_n \\ \tilde{\tau}_n \end{bmatrix}.$$

The goal is to find $a_{n+1} \in \mathbb{C}^{n+2}$ such that it satisfies the orthogonality condition, with $\tau_{n+1} \neq 0$, i.e., no breakdown,

$$M_{n+1} \begin{bmatrix} a_{n+1} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tau_{n+1} \end{bmatrix}.$$

It is easy to verify that $\eta_n a_{n+1} = Z_{n+1} P_{n+1} \tilde{a}_n - \gamma_n a_n$, with $\gamma_n = \frac{\tilde{\alpha}_n}{\tau_n}$, will satisfy the orthogonality condition. Writing this in terms of Laurent polynomials provides $\eta_n a_{n+1}(z) = z \tilde{a}_n(z) - \gamma_n a_n(z)$ and the recurrence relation for odd indices has been shown.

Similarly for $\tilde{a}_{n+1}(z)$, consider

$$\tilde{M}_{n+1} \begin{bmatrix} \tilde{a}_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{\tau}_n \\ \tilde{\alpha}_n \end{bmatrix} \quad \text{and} \quad \tilde{M}_{n+1} \tilde{Z}_{n+1} P_{n+1} \begin{bmatrix} a_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \alpha_n \\ \tau_n \end{bmatrix}.$$

Hence, $\tilde{\eta}_n \tilde{a}_{n+1}(z) = z^{-1} a_n(z) - \tilde{\gamma}_n \tilde{a}_n(z)$, with $\tilde{\gamma}_n = \frac{\alpha_n}{\tilde{\tau}_n}$, satisfies the proposed recurrence relation. For even indices a small adjustment must be made to the derivation. Consider

$$M_{n+2} \begin{bmatrix} a_{n+1} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tau_{n+1} \\ \alpha_{n+1} \end{bmatrix} \quad \text{and} \quad M_{n+2} P_{n+2} \begin{bmatrix} \tilde{a}_{n+1} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{\alpha}_{n+1} \\ \tilde{\tau}_{n+1} \end{bmatrix},$$

and $\eta_{n+1} a_{n+2}(z) = \tilde{a}_{n+1}(z) - \gamma_{n+1} a_{n+1}(z)$, $\gamma_{n+1} = \frac{\tilde{\alpha}_{n+1}}{\tau_{n+1}}$. Similarly $\tilde{a}_{n+2}(z)$ can be shown to satisfy $\tilde{\eta}_{n+1} a_{n+2}(z) = \tilde{a}_{n+1}(z) - \tilde{\gamma}_{n+1} a_{n+1}(z)$, $\tilde{\gamma}_{n+1} = \frac{\alpha_{n+1}}{\tilde{\tau}_{n+1}}$.

The proof of the recurrence relations for $b_i(z)$ can be done in a similar way. $\square$

Remark 1. Part of the proof of Theorem 5 can be done using matrix theory and provides new insight. Once the recurrence relations for $a_i(z)$ are known, the recurrence relations for $b_i(z)$ can be immediately derived from the moment matrix. The moment matrix $M = S^H K$ is related to $a_i(z)$, in the sense that $a_i(A)v$ lives in the space spanned by K and is orthogonal to the space spanned by S . The dual, an element of the space spanned by S and orthogonal to space spanned by K , is $b_i(z)$ which relates to $M^H = K^H S$. For $\tilde{a}_i(z)$ and $\tilde{b}_i(z)$, the related moment matrices are $\tilde{M} = M^\top$ and $\tilde{M}^H = \tilde{M}$. Let $R_n \in \mathbb{C}^{(n+1) \times (n+1)}$ be the matrix formed by the recurrence coefficients of $a_i(z)$, $i = 0, 1, \dots, n$, and $\tilde{R}_n \in \mathbb{C}^{(n+1) \times (n+1)}$ formed by those of $\tilde{a}_i(z)$, $i = 0, 1, \dots, n$. Then $M_n R_n = L_n$, L_n lower triangular and $\tilde{M}_n \tilde{R}_n = \tilde{L}_n$, also lower triangular. In other words, we have two LR-factorizations of the moment matrix M , since, $\tilde{M}_n^\top = M_n = \tilde{R}_n^\top \tilde{L}_n^\top$ and $M_n = L_n R_n^{-1}$. Because the LR-factorization of a strongly nonsingular matrix (guaranteed by the no-breakdown assumption) is essentially unique, there exists a normalization such that $\tilde{R}_n^\top = L_n$ and $\tilde{L}_n^\top = R_n$. Note that the LR-factorisation of a moment matrix is connected to the orthogonalisation of the bases constructing this moment matrix [3, p.44]. From this equality between the LR-factors of M and $\tilde{M}$ and their reappearance in the analysis of $b_i(z)$ and $\tilde{b}_i(z)$, through M^H and $\tilde{M}^H$, the recurrence coefficients for these Laurent polynomials can be immediately retrieved. More precisely, for $b_i(z)$ the recurrence coefficients are represented by L_n^{-H} , since, $M_n^H L_n^{-H} = R_n^{-H}$. Finally, $L_n^{-H} = L_n^{-\top} = \tilde{R}_n$, so the recurrence coefficients of $b_i(z)$ are simply the complex conjugate of the recurrence coefficients of $\tilde{a}_i(z)$.

2.4 Connection with CMV

To retrieve the results reported by Watkins [10], it suffices to consider the same normalized starting vector for all spaces $v = w = h$ and a unitary matrix U . The following corollaries summarize the results for the CMV which are given above in the more general case.

For the CMV, the two pairs of four-term recurrence relations from Theorem 1 collapse into one pair of recurrence relations. The corresponding projected matrix is unitary. These results are given in Corollary 1 and 2, respectively.

Corollary 1. Consider a unitary matrix $U \in \mathbb{C}^{m \times m}$ and $h \in \mathbb{C}^m$. Then, with normalization of η_i such that $\langle v_i, v_i \rangle = 1$,

$$\begin{aligned} \eta_{2k+1, 2k} v_{2k+1} &= U v_{2k-1} - \alpha_{2k-2, 2k} v_{2k-2} - \alpha_{2k-1, 2k} v_{2k-1} - \alpha_{2k, 2k} v_{2k}, \\ \eta_{2k+2, 2k+1} v_{2k+2} &= U^H v_{2k} - \alpha_{2k-1, 2k+1} v_{2k-1} - \alpha_{2k, 2k+1} v_{2k} - \alpha_{2k+1, 2k+1} v_{2k+1}. \end{aligned}$$

Corollary 2. Consider a unitary matrix $U \in \mathbb{C}^{m \times m}$, $h \in \mathbb{C}^m$ and an orthogonal basis $V_l \in \mathbb{C}^{m \times (l+1)}$ for $\mathcal{K}_l(U, h)$. Then the orthogonal projection of U onto $\mathcal{K}_l(U, h)$,

$$V_l^H U V_l = Z_l, \quad (28)$$

is a unitary matrix $Z_l \in \mathbb{C}^{(l+1) \times (l+1)}$ with pentadiagonal structure.

For the two-term recurrence relations, given in Theorem 3, the four pairs of recurrence relations collapse into two pairs. The coefficients also simplify, since $\tilde{\gamma} = \bar{\gamma}$. The result is stated in Corollary 3. The related matrix pencil of the projected matrix consists of two unitary tridiagonal matrices, Corollary 4 states this result.

Corollary 3. Consider a unitary matrix $U \in \mathbb{C}^{m \times m}$ and $h \in \mathbb{C}^m$. Then, with normalization of η_i and $\tilde{\eta}_i$ such that $\langle v_i, v_i \rangle = 1$ and $\langle \tilde{v}_i, \tilde{v}_i \rangle = 1$, the recurrence relations (12) - (19) become

$$\begin{aligned}\eta_{2k} v_{2k+1} &= U \tilde{v}_{2k} - \gamma_{2k} v_{2k}, \\ \tilde{\eta}_{2k} \tilde{v}_{2k+1} &= U^H v_{2k} - \tilde{\gamma}_{2k} \tilde{v}_{2k},\end{aligned}$$

and

$$\begin{aligned}\eta_{2k+1} v_{2k+2} &= \tilde{v}_{2k+1} - \gamma_{2k+1} v_{2k+1}, \\ \tilde{\eta}_{2k+1} \tilde{v}_{2k+2} &= v_{2k+1} - \tilde{\gamma}_{2k+1} \tilde{v}_{2k+1}.\end{aligned}$$

The vectors $v_i, \tilde{v}_i, i = 0, 1, \dots, l$, form orthogonal bases for $\mathcal{K}_l(U, h)$ and $\mathcal{S}_l(U, h)$, respectively.

Corollary 4. Consider a unitary matrix $U \in \mathbb{C}^{m \times m}$, a vector $h \in \mathbb{C}^m$ and an orthogonal basis $V_l \in \mathbb{C}^{m \times (l+1)}$ for $\mathcal{K}_l(U, h)$. The matrix pencil of recurrence coefficients $(\hat{T}_l, \hat{S}_l)$, with $\hat{T}_l, \hat{S}_l \in \mathbb{C}^{(l+1) \times l}$ satisfying

$$AV_{l+1}\hat{S}_l = V_{l+1}\hat{T}_l,$$

can be represented by two unitary tridiagonal matrices with the same sparsity structure as in Theorem 4.

The recurrence relations for the Laurent polynomials simplify in a similar manner, stated in Corollary 5.

Corollary 5. Consider Laurent polynomials $a_i(z) \in \mathcal{F}_i(z)$ and $\tilde{a}_i(z) \in \mathcal{G}_i(z)$. If these are constructed as

$$\begin{aligned}\eta_{2k} a_{2k+1}(z) &= z \tilde{a}_{2k}(z) - \gamma_{2k} a_{2k}(z), \\ \tilde{\eta}_{2k} \tilde{a}_{2k+1}(z) &= z^{-1} a_{2k}(z) - \tilde{\gamma}_{2k} \tilde{a}_{2k}(z), \\ \eta_{2k+1} a_{2k+2}(z) &= \tilde{a}_{2k+1}(z) - \gamma_{2k+1} a_{2k+1}(z), \\ \tilde{\eta}_{2k+1} \tilde{a}_{2k+2}(z) &= a_{2k+1}(z) - \tilde{\gamma}_{2k+1} \tilde{a}_{2k+1}(z),\end{aligned}$$

where $\gamma_{2k} = \langle z \tilde{a}_{2k}(z), a_{2k}(z) \rangle$, $\gamma_{2k+1} = \langle \tilde{a}_{2k+1}(z), a_{2k+1}(z) \rangle$, $\tilde{\gamma}_i = \bar{\gamma}_i$ and $\eta_i, \tilde{\eta}_i$ are chosen such that $\langle v_i, v_i \rangle = 1$, $\langle \tilde{v}_i, \tilde{v}_i \rangle = 1$, respectively. Then the sequence $\{a_i(z)\}_i$ is a sequence of orthogonal Laurent polynomials. That is, $\langle a_i(z), a_j(z) \rangle = \delta_{ij}$, with respect to the inner product from Definition 1. Similarly for the sequence $\{\tilde{a}_i(z)\}_i$.

Also note that the moment matrix is Hermitian and positive definite. Hence, it allows for a Cholesky factorization which means $L_n = R_n^H$, i.e., coefficients are the same. This implies that, under suitable choice of normalization and starting vector, the biorthogonal bases collapse into one orthogonal basis.

3 Numerical behaviour

The numerical behaviour of the proposed four- and two-term recurrence relations from Theorem 1 and Theorem 3 is analysed. The matrices $A \in \mathbb{C}^{m \times m}$ used are restricted to well-conditioned normal matrices. Testing the recurrence relations with these matrices will shed some light on the stability of the methods. We are interested in the biorthogonality of the generated bases and how accurate the projection matrices represent the projection. Biorthogonality of the generated bases $V_n \in \mathbb{C}^{m \times (n+1)}$ and $W_n \in \mathbb{C}^{m \times (n+1)}$ for the Krylov subspaces $\mathcal{K}_n(A, v)$ and $\mathcal{S}_n(A^H, v)$ is quantified by

$$\|W_n^H V_n - I\|_2,$$

with I the unit matrix of appropriate size. This error will be called the biorthogonality error. The quality of the projection matrix Z and projection matrix pencil (T, S) will be monitored by the projection error, defined as

$$\frac{\|AV_n - V_{n+1}Z_{n+1}\|_2}{\|A\|_2}$$

and

$$\frac{\|AV_n S_n - V_n T_n\|_2}{\|A\|_2},$$

respectively. The projection matrix and projection matrix pencil are related to the matrices of recurrence coefficients from Theorem 2 and Theorem 4, respectively. Two other metrics are useful in order to interpret the results. These are the condition number of the matrix A , denoted by $\kappa(A)$, and the growth factor, defined, for the two- and four-term recurrence relation respectively, as

$$\rho := \frac{\max(\max(|T|, |S|))}{\max(|A|)} \text{ and } \rho := \frac{\max(|Z|)}{\max(|A|)}.$$

The growth factor provides a metric for stability. Throughout this section a modest size of matrices is chosen, a dimension of $m = 200$. This can be done without loss of generality, larger matrices (with the same properties) do inherently cause larger numerical errors, however the numerical behaviour remains similar.

3.1 Unitary matrices

Consider the case corresponding to the CMV-decomposition, $U \in \mathbb{C}^{m \times m}$ is a unitary matrix and the starting vectors for the Krylov subspaces are equal, i.e., $v = w = h \in \mathbb{C}^m$. Let $m = 200$ and h be a random vector. Both recurrence relations have a low biorthogonality and projection error, shown in Figure 1. When the dimension of the subspaces, $n + 1$, nears the dimension of the matrix, m , biorthogonality is lost more rapidly since the Ritz values (i.e., eigenvalues of the projection matrix) start to accurately approximate the eigenvalues of A . Furthermore, all projection matrices, Z , S and T are close to unitary. Hence, we conclude that for a unitary matrix and same starting vectors, we retrieve the CMV case.

Figure 1: Biorthogonality and projection error, respectively left and right, for a unitary matrix $U \in \mathbb{C}^{200 \times 200}$ and same starting vectors. Two-term recurrence relation in blue and four-term recurrence relation in red.

3.2 Scaled and shifted unitary matrices

Consider scaled and shifted unitary matrices, i.e., for a unitary matrix $U \in \mathbb{C}^{m \times m}$ and scalars $\mu, \omega \in \mathbb{R}$, $A = (\mu U + \omega I) \in \mathbb{C}^{m \times m}$. Starting vectors are equal for all Krylov subspaces. Figure 2 shows the biorthogonality

and projection errors for $\mu = 1.1$ and $\omega = 0$. Both errors are still small, however compared to the unitary case, shown in Figure 1, they are larger. The projection error increases steadily from $n = 55$ and $n = 120$, for the two- and four-term recurrence relations, respectively. This can be (at least partially) explained by the increasing growth factor ρ , which is approximately $\rho(n) = \mu^n$. Figure 3 shows the errors for $\mu = 1$ and $\omega = 0.1$. The two-term recurrence relation performs better than the four-term recurrence relation, especially in terms of projection error.

Figure 2: Biorthogonality and projection error, respectively left and right, for a scaled unitary matrix $\mu U \in \mathbb{C}^{200 \times 200}$, with $\mu = 1.1$ and same starting vectors. Two-term recurrence relation in blue and four-term recurrence relation in red.

Figure 3: Biorthogonality and projection error, respectively left and right, for a shifted unitary matrix $(U + \omega I) \in \mathbb{C}^{200 \times 200}$, with $\omega = 0.1$ and same starting vectors. Two-term recurrence relation in blue and four-term recurrence relation in red.

3.3 General normal matrices

Consider a normal matrix $A \in \mathbb{C}^{m \times m}$ with condition number $\kappa(A) = 10$ and starting vectors $v, w \in \mathbb{C}^m$ not necessarily equal. The errors are shown in Figure 4. The two- and four-term recurrence relations perform similar for both metrics. Biorthogonality is lost quickly and there is no Ritz value which approximates an eigenvalue accurately. Hence, this loss of biorthogonality is due to the recurrence relations themselves. Figure 5 shows the magnitude of the elements in the moment matrix $W_{20}^H V_{20} - I$. There is clearly a pattern visible, however further research into the numerical properties of the recurrence relation must be done in order to interpret this.

Figure 4: Biorthogonality and projection error, respectively left and right, for a normal matrix $A \in \mathbb{C}^{200 \times 200}$, with condition number $\kappa(A) = 10$. Two-term recurrence relation in blue and four-term recurrence relation in red.

Figure 5: Magnitude (base 10) of the elements appearing in the moment matrix $W_{20}^H V_{20} - I$ for the two- and four-term recurrence relation on the left and right, respectively. Bases V, W are constructed for a normal matrix A with $\kappa(A) = 10$.

3.4 Conclusion

The numerical experiments verify the validity of the recurrence relations. The two-term recurrence relation performs better than the four-term recurrence relation. Biorthogonality can be lost quickly, further research must be done in order to understand and improve this. Reorthogonalization strategies can improve the biorthogonality of the generated bases.

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