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KRYLOV SUBSPACES ASSOCIATED WITH HIGHER-ORDER LINEAR DYNAMICAL SYSTEMS

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Abstract.

A standard approach to model reduction of large-scale higher-order linear dynamical systems is to rewrite the system as an equivalent first-order system and then employ Krylov-subspace techniques for model reduction of first-order systems. This paper presents some results about the structure of the block-Krylov subspaces induced by the matrices of such equivalent first-order formulations of higher-order systems. Two general classes of matrices, which exhibit the key structures of the matrices of first-order formulations of higher-order systems, are introduced. It is proved that for both classes, the block-Krylov subspaces induced by the matrices in these classes can be viewed as multiple copies of certain subspaces of the state space of the original higher-order system.

AMS subject classification (2000): 65F30, 15A57, 65P99, 41A21.

Key words: Krylov subspace, linear dynamical system, second-order system, higher-order system, model reduction.

1 Introduction.

In recent years, Krylov-subspace methods, especially the Lanczos algorithm and the Arnoldi process, have become popular tools for model reduction of large-scale time-invariant linear dynamical systems; we refer the reader to the survey papers [7, 8, 2, 9], and the references given there. Krylov-subspace techniques can be applied directly only to first-order linear dynamical systems. However, there are important applications, for example in VLSI circuit simulation [20, 10, 11], structural dynamics [16, 5, 19], and computational electromagnetics [24], that lead to second-order, or even general higher-order, linear dynamical systems.

The standard approach to employing Krylov-subspace methods for model reduction of a second-order or higher-order system is to first rewrite the system as an equivalent first-order system, and then apply Krylov-subspace techniques for reduced-order modeling of first-order systems. At first glance, there are two disadvantages of this standard approach. First, the second-order or higher-order structure is not preserved by a straightforward application of Krylov-subspace methods to the first-order formulation. Second, the computational cost increases due to the fact that the state-space dimension of the first-order formulation is l times the state-space dimension of the original l -th-order system. A partial

remedy of the first problem is to use certain structure-preserving projections, as described in the recent papers [23, 10, 22, 11, 4, 18]. However, the structure-preserving property of these approaches comes at the expense of reduced approximation quality of the resulting models. To address the second problem, at least for the special case of second-order systems, various authors have proposed to directly generate basis vectors of certain subspaces of the state space of the second-order system, rather than basis vectors of the Krylov subspaces of the first-order formulation; see, e.g., [3, 14, 17, 19, 25].

The purpose of this paper is to shed some light on the second problem and to present some results on the special structures of the block-Krylov subspaces induced by the matrices of equivalent first-order formulations of general higher-order time-invariant linear dynamical systems and of certain systems of first-order integro-differential-algebraic equations. More precisely, we introduce two classes of structured matrices, which include the matrices of these first-order formulations as special cases. As our main results, we show that the block-Krylov subspaces induced by the matrices in these classes exhibit special structures. Roughly speaking, for both classes, the associated structured block-Krylov subspaces consist of multiple copies of certain subspaces of the state space of the original higher-order system.

These results have several implications. First, they show that in order to use Krylov subspace-type information for second-order or higher-order systems, there is really no need to develop new special Krylov-subspace methods. Indeed, since all this information is already contained in the standard Krylov subspaces induced by the matrices of equivalent first-order formulations, one can simply employ existing Krylov-subspace techniques. Second, since each of these standard first-order Krylov subspaces simply consists of multiple, say l , copies of the same subspace of a lower-dimensional space, the costs of the matrix-vector products can be reduced by a factor of l . Third, many of the existing solutions for the more involved problems (such as the need for deflation) that arise in the case of block-Krylov subspaces can simply be reused, and there is no need to reconsider all these issues.

The remainder of the paper is organized as follows. In Section 2, we briefly review the notion of block-Krylov subspaces. In Section 3, we introduce two classes of matrices, and we state our main results about the special structures of the block-Krylov subspaces associated with these two classes. In Section 4, we present proofs of these main results. In Section 5, we consider higher-order linear dynamical systems, and we show how certain model-reduction approaches lead to matrices that are special instances of the first class of matrices introduced in Section 3. In Section 6, we study systems of first-order integro-differential-algebraic equations, and we show how model reduction leads to matrices that are special instances of the second class of matrices introduced in Section 3. Finally, in Section 7, we make some concluding remarks.

Throughout this paper the following notation is used. The set of real and complex numbers is denoted by \mathbb{R} and \mathbb{C} , respectively. Unless stated otherwise, all vectors and matrices are allowed to have real or complex entries. For a matrix

$A = [a_{jk}] \in \mathbb{C}^{m \times n}$, we denote by $A^H := [\overline{a_{kj}}] \in \mathbb{C}^{n \times m}$ its conjugate transpose. For any two matrices $A = [a_{jk}] \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{p \times q}$,

$$A \otimes B := [a_{jk}B] \in \mathbb{C}^{mp \times nq}$$

is the Kronecker product [13, 21] of A and B . The $n \times n$ identity matrix is denoted by I_n and the zero matrix by 0. If the dimension of I_n is apparent from the context, we drop the index and simply use I . The actual dimension of 0 will always be apparent from the context.

2 Block-Krylov subspaces.

We use the notion of block-Krylov subspaces that was introduced in [1] in connection with a band Lanczos process for multiple starting vectors. In this section, we briefly review the definition of block-Krylov subspaces from [1].

In the following, let

$$(2.1) \quad \mathcal{M} \in \mathbb{C}^{N \times N} \quad \text{and} \quad \mathcal{R} = [r_1 \ r_2 \ \cdots \ r_m] \in \mathbb{C}^{N \times m}$$

be given matrices. The $N \times mN$ matrix

$$(2.2) \quad [\mathcal{R} \ \mathcal{M}\mathcal{R} \ \mathcal{M}^2\mathcal{R} \ \cdots \ \mathcal{M}^{N-1}\mathcal{R}]$$

is called the *block-Krylov matrix* induced by \mathcal{M} and \mathcal{R} .

2.1 The case of exact deflation.

Let $N_0 (\leq N)$ denote the rank of the block-Krylov matrix (2.2). Hence only N_0 of the mN columns of (2.2) are linearly independent. Such a set of N_0 linearly independent columns can be constructed by scanning the columns of (2.2) from left to right and deleting each column that is linearly dependent on earlier columns. This process of deleting linearly dependent columns is called *exact deflation*. By the structure of the block-Krylov matrix (2.2), a column $\mathcal{M}^{k-1}r_i$ being linearly dependent on earlier columns implies that all columns $\mathcal{M}^j r_i$, $k \leq j \leq N-1$, are also linearly dependent on earlier columns. Consequently, applying exact deflation to (2.2) results in a matrix of the form

$$(2.3) \quad \mathcal{V}(\mathcal{M}, \mathcal{R}) := [\mathcal{R}_1 \ \mathcal{M}\mathcal{R}_2 \ \mathcal{M}^2\mathcal{R}_3 \ \cdots \ \mathcal{M}^{k_0-1}\mathcal{R}_{k_0}] \in \mathbb{C}^{N \times N_0}.$$

Here, for each $k = 1, 2, \dots, k_0$, $\mathcal{R}_k \in \mathbb{C}^{N \times m_k}$ is a submatrix of $\mathcal{R}_{k-1} \in \mathbb{C}^{N \times m_{k-1}}$, with $\mathcal{R}_k \neq \mathcal{R}_{k-1}$ if, and only if, exact deflation occurs within the k -th Krylov block $\mathcal{M}^{k-1}\mathcal{R}$ in (2.2). (For $k = 1$, we set $\mathcal{R}_0 = \mathcal{R}$ and $m_0 = m$.) For later use, we remark that

$$(2.4) \quad \mathcal{R}_k = \mathcal{R}_{k-1}E_k, \quad E_k \in \mathbb{C}^{m_{k-1} \times m_k}, \quad m_k \leq m_{k-1},$$

where E_k is the *deflated identity matrix* obtained from $I_{m_{k-1}}$ by deleting those $m_{k-1} - m_k$ columns corresponding to exact deflation within the k -th Krylov block.

By construction, the matrix (2.3) has full column rank N_0 . For $1 \leq n \leq N_0$, the n -th *block-Krylov subspace* (induced by \mathcal{M} and \mathcal{R}), $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$, is defined as the n -dimensional subspace of \mathbb{C}^N spanned by the first n columns of (2.3). We say that

$$\mathcal{V} = [v_1 \ v_2 \ \cdots \ v_{N_0}] \in \mathbb{C}^{N \times N_0}$$

is a *basis matrix* of the block-Krylov subspaces induced by \mathcal{M} and \mathcal{R} if

$$\mathcal{K}_n(\mathcal{M}, \mathcal{R}) = \text{span}[v_1 \ v_2 \ \cdots \ v_n] \quad \text{for all } n = 1, 2, \dots, N_0.$$

Note that the matrix $\mathcal{V}(\mathcal{M}, \mathcal{R})$ defined in (2.3) is a particular instance of a basis matrix. Furthermore, any two basis matrices \mathcal{V}_1 and \mathcal{V}_2 of the block-Krylov subspaces induced by \mathcal{M} and \mathcal{R} are connected by a relation of the form

$$(2.5) \quad \mathcal{V}_1 = \mathcal{V}_2 \mathcal{U},$$

where \mathcal{U} is a nonsingular and upper triangular matrix.

Lanczos- and Arnoldi-type algorithms for the actual construction of basis matrices of block-Krylov subspaces can be found in [1] and [9].

2.2 *Inexact deflation.*

In the above construction of block-Krylov subspaces, we performed only exact deflation. In an actual algorithm for constructing a basis matrix of the block-Krylov subspaces induced by \mathcal{M} and \mathcal{R} in finite-precision arithmetic, one also needs to delete vectors that are in some sense “almost” linearly dependent on earlier vectors. The deletion of such almost linearly dependent vectors is called *inexact deflation*. For example, the Lanczos- and Arnoldi-type algorithms in [1] and [9] have simple built-in procedures for both exact and inexact deflation.

It turns out that the construction of block Krylov subspaces described in Subsection 2.1 can be extended to the more general case when exact and inexact deflations are performed. The deflated matrix (2.3) is now obtained by deleting from the block-Krylov matrix (2.2) those columns that are linearly or almost linearly dependent on columns to their left. In the general case, N_0 is now simply defined as the number of columns of the resulting deflated matrix (2.3). Note that N_0 is less than or equal to the rank of the block-Krylov matrix (2.2), with equality only if no inexact deflation occurs. Based on the deflated matrix (2.3), block-Krylov subspaces and basis matrices of these subspaces are defined in the same way as in Subsection 2.1. However, note that the resulting block-Krylov subspaces are in general different from the block-Krylov subspaces obtained with exact deflation only.

The main results of this paper, namely Theorems 3.1 and 3.2 below, hold true for the general case of exact and inexact deflations, provided that the matrices \mathcal{R}_k in (2.3) still satisfy relations of the form (2.4). This is the case for the built-in deflation procedures of the Lanczos- and Arnoldi-type algorithms in [1] and [9]. Thus, in the following, we always assume that the matrices \mathcal{R}_k in (2.3) indeed satisfy relations of the form (2.4).

3 Main results.

In this section, we introduce two classes of matrices \mathcal{M} and \mathcal{R} , and we state our main results about the special structures of the block-Krylov subspaces associated with these two classes. Proofs of these results are given in Section 4 below.

3.1 Case I.

In this subsection, we assume that the matrices (2.1) are of the form

$$(3.1) \quad \begin{aligned} \mathcal{M} &= (c \otimes I_{n_0}) [M^{(1)} \quad M^{(2)} \quad \cdots \quad M^{(l)}] + \Sigma \otimes I_{n_0}, \\ \mathcal{R} &= c \otimes R, \end{aligned}$$

where

$$(3.2) \quad \begin{aligned} &M^{(i)} \in \mathbb{C}^{n_0 \times n_0}, \quad i = 1, 2, \dots, l, \quad R \in \mathbb{C}^{n_0 \times m}, \\ c &= \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_l \end{bmatrix} \in \mathbb{C}^l, \quad \text{and} \quad \Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1l} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2l} \\ \vdots & \vdots & & \vdots \\ \sigma_{l1} & \sigma_{l2} & \cdots & \sigma_{ll} \end{bmatrix} \in \mathbb{C}^{l \times l}. \end{aligned}$$

We assume that

$$(3.3) \quad c_i \neq 0, \quad i = 1, 2, \dots, l.$$

Note that $\mathcal{M} \in \mathbb{C}^{N \times N}$ and $\mathcal{R} \in \mathbb{C}^{N \times m}$, where

$$(3.4) \quad N := ln_0.$$

Our main result about the structure of the block-Krylov subspaces associated with the class of matrices (3.1) is as follows.

THEOREM 3.1. *Let \mathcal{M} and \mathcal{R} be matrices of the form (3.1) and (3.2), and assume that (3.3) is satisfied. Let $\mathcal{V} \in \mathbb{C}^{N \times N_0}$ be any basis matrix of the block-Krylov subspaces induced by \mathcal{M} and \mathcal{R} . Then, \mathcal{V} can be represented in the form*

$$(3.5) \quad \mathcal{V} = \begin{bmatrix} W U^{(1)} \\ W U^{(2)} \\ \vdots \\ W U^{(l)} \end{bmatrix},$$

where $W \in \mathbb{C}^{n_0 \times N_0}$ and, for each $i = 1, 2, \dots, l$, $U^{(i)} \in \mathbb{C}^{N_0 \times N_0}$ is nonsingular and upper triangular.

The result of Theorem 3.1 can be interpreted as follows. Let

$$(3.6) \quad S_n := \text{span}[w_1 \quad w_2 \quad \cdots \quad w_n] \subseteq \mathbb{C}^{n_0}, \quad n = 1, 2, \dots, N_0,$$

denote the sequence of subspaces spanned by the leading columns of the matrix

$$(3.7) \quad W = [w_1 \quad w_2 \quad \cdots \quad w_{N_0}] \in \mathbb{C}^{n_0 \times N_0}.$$

In view of (3.5), for each $n = 1, 2, \dots, N_0$, the n -th block-Krylov subspace $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$, even though it is a subspace in \mathbb{C}^N , consists of l ‘copies’ of the same subspace S_n , which is a subspace of only \mathbb{C}^{n_0} , where, by (3.4), $n_0 = N/l$. We stress that, in general, S_n is not a block-Krylov subspace.

3.2 Case II.

In this subsection, we assume that the matrices (2.1) are of the form

$$(3.8) \quad \mathcal{M} = \begin{bmatrix} C^{(1)} \\ C^{(2)} \\ \vdots \\ C^{(l)} \end{bmatrix} [M^{(1)} \quad M^{(2)} \quad \dots \quad M^{(l)}] + \begin{bmatrix} \sigma_1 I_{n_1} & 0 & \dots & 0 \\ 0 & \sigma_2 I_{n_2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \sigma_l I_{n_l} \end{bmatrix},$$

$$\mathcal{R} = \begin{bmatrix} C^{(1)} \\ C^{(2)} \\ \vdots \\ C^{(l)} \end{bmatrix} R,$$

where

$$(3.9) \quad \begin{aligned} C^{(i)} &\in \mathbb{C}^{n_i \times n_0}, \quad M^{(i)} \in \mathbb{C}^{n_0 \times n_i}, \quad \sigma_i \in \mathbb{C}, \quad i = 1, 2, \dots, l, \\ \text{and } R &\in \mathbb{C}^{n_0 \times m}. \end{aligned}$$

Note that $\mathcal{M} \in \mathbb{C}^{N \times N}$ and $\mathcal{R} \in \mathbb{C}^{N \times m}$, where

$$N := n_1 + n_2 + \dots + n_l.$$

Our main result about the structure of the block-Krylov subspaces associated with the class of matrices (3.8) is as follows.

THEOREM 3.2. *Let \mathcal{M} and \mathcal{R} be matrices of the form (3.8) and (3.9). Let $\mathcal{V} \in \mathbb{C}^{N \times N_0}$ be any basis matrix of the block-Krylov subspaces induced by \mathcal{M} and \mathcal{R} . Then, \mathcal{V} can be represented in the form*

$$(3.10) \quad \mathcal{V} = \begin{bmatrix} C^{(1)} W U^{(1)} \\ C^{(2)} W U^{(2)} \\ \vdots \\ C^{(l)} W U^{(l)} \end{bmatrix},$$

where $W \in \mathbb{C}^{n_0 \times N_0}$ and, for each $i = 1, 2, \dots, l$, $U^{(i)} \in \mathbb{C}^{N_0 \times N_0}$ is nonsingular and upper triangular.

The result of Theorem 3.2 can be interpreted as follows. Let $S_n \subseteq \mathbb{C}^{n_0}$, $n = 1, 2, \dots, N_0$, again denote the sequence of subspaces spanned by the leading columns of the matrix W ; as defined in (3.6) and (3.7). In view of (3.10), for each $n = 1, 2, \dots, N_0$, the n -th block-Krylov subspace $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$, even though it is a subspace in \mathbb{C}^N , consists of l ‘copies’ of the $C^{(i)}$ -multiples, $i = 1, 2, \dots, l$, of the same subspace S_n , which is a subspace of \mathbb{C}^{n_0} .

4 Proofs

In this section, we present proofs of Theorems 3.1 and 3.2.

4.1 Proof of Theorem 3.1.

Let \mathcal{V} be a given basis matrix of the block Krylov subspaces induced by \mathcal{M} and \mathcal{R} . We need to show that there exists a matrix W and nonsingular upper triangular matrices $U^{(i)}$, $i = 1, 2, \dots, l$, such that (3.5) holds true.

Recall that any two basis matrices are connected by a relation of the form (2.5), where U is a nonsingular and upper triangular matrix. Therefore, without loss of generality, we may assume that

$$(4.1) \quad \mathcal{V} = \mathcal{V}(\mathcal{M}, \mathcal{R})$$

is the particular basis matrix defined in (2.3). Furthermore, we partition any possible candidate matrices W and $U^{(i)}$, $i = 1, 2, \dots, l$, according to the block sizes of $\mathcal{V}(\mathcal{M}, \mathcal{R})$ in (2.3). More precisely, we set

$$(4.2) \quad W = [W_1 \quad W_2 \quad \cdots \quad W_{k_0}],$$

$$U^{(i)} = \begin{bmatrix} U_{11}^{(i)} & U_{12}^{(i)} & \cdots & U_{1k_0}^{(i)} \\ 0 & U_{22}^{(i)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & U_{k_0 k_0}^{(i)} \end{bmatrix}, \quad i = 1, 2, \dots, l,$$

with subblocks $W_k \in \mathbb{C}^{n_0 \times m_k}$ and nonsingular upper triangular diagonal blocks $U_{kk}^{(i)} \in \mathbb{C}^{m_k \times m_k}$ for all $i = 1, 2, \dots, l$ and $k = 1, 2, \dots, k_0$. Inserting (4.1) and (4.2) into (3.5), it follows that the desired relation (3.5) holds true if, and only if,

$$(4.3) \quad \mathcal{M}^{k-1} \mathcal{R}_k = \begin{bmatrix} \sum_{j=1}^k W_j U_{jk}^{(1)} \\ \sum_{j=1}^k W_j U_{jk}^{(2)} \\ \vdots \\ \sum_{j=1}^k W_j U_{jk}^{(l)} \end{bmatrix}, \quad k = 1, 2, \dots, k_0.$$

Therefore, it remains to construct the subblocks in (4.2) such that (4.3) is satisfied. To this end, we define these subblocks recursively as follows.

For each $k = 1, 2, \dots, k_0$, we set

$$(4.4) \quad U_{jk}^{(i)} := \begin{cases} \left(\sum_{t=1}^l \sigma_{i,t} U_{j,k-1}^{(t)} \right) E_k, & \text{for } j = 1, 2, \dots, k-1, \\ c_i I_{m_k}, & \text{for } j = k, \end{cases}$$

for all $i = 1, 2, \dots, l$, and

$$(4.5) \quad W_k := \begin{cases} RE_1, & \text{if } k = 1, \\ \left(\sum_{i=1}^l M^{(i)} \left(\sum_{j=1}^{k-1} W_j U_{j,k-1}^{(i)} \right) \right) E_k, & \text{if } k > 1. \end{cases}$$

Here, the matrices E_k are the ones from (2.4). We remark that, in view of assumption (3.3), the subblocks $U_{kk}^{(i)}$ in (4.4) are all nonsingular. Moreover, they are all diagonal and thus, in particular, upper triangular.

Using induction on k , we now show that the subblocks (4.4) and (4.5) indeed satisfy (4.3). Recall from (3.1) that $\mathcal{R} = c \otimes R$ and from (2.4) (for $k = 1$) that $\mathcal{R}_1 = \mathcal{R}E_1$. Together with the definitions of $U_{11}^{(i)}$, $i = 1, 2, \dots, l$, in (4.4) and of W_1 in (4.5), it follows that

$$\mathcal{R}_1 = c \otimes (RE_1) = \begin{bmatrix} c_1 RE_1 \\ c_2 RE_1 \\ \vdots \\ c_l RE_1 \end{bmatrix} = \begin{bmatrix} W_1 U_{11}^{(1)} \\ W_1 U_{11}^{(2)} \\ \vdots \\ W_1 U_{11}^{(l)} \end{bmatrix}.$$

This is just (4.3) for $k = 1$. Let $1 < k \leq k_0$ and assume that (4.3) holds true for $k - 1$. Then, by multiplying the relation (4.3) (with k replaced by $k - 1$) from the left by the matrix \mathcal{M} from (3.1), it follows that

$$\begin{aligned} \mathcal{M}^{k-1} \mathcal{R}_{k-1} &= \mathcal{M} \left(\mathcal{M}^{k-2} \mathcal{R}_{k-1} \right) \\ &= (c \otimes I_{n_0}) \left(\sum_{i=1}^l M^{(i)} \left(\sum_{j=1}^{k-1} W_j U_{j,k-1}^{(i)} \right) \right) + \begin{bmatrix} \sum_{t=1}^l \sigma_{1,t} \sum_{j=1}^{k-1} W_j U_{j,k-1}^{(t)} \\ \sum_{t=1}^l \sigma_{2,t} \sum_{j=1}^{k-1} W_j U_{j,k-1}^{(t)} \\ \vdots \\ \sum_{t=1}^l \sigma_{l,t} \sum_{j=1}^{k-1} W_j U_{j,k-1}^{(t)} \end{bmatrix}. \end{aligned}$$

Multiplying this relation from the right by the matrix E_k from (2.4) and using the definitions of $U_{jk}^{(i)}$, $i = 1, 2, \dots, l$, $j = 1, 2, \dots, k$, in (4.4) and of W_k in (4.5), we obtain

$$\begin{aligned} \mathcal{M}^{k-1} \mathcal{R}_k &= \mathcal{M}^{k-1} \mathcal{R}_{k-1} E_k \\ &= \begin{bmatrix} W_k U_{kk}^{(1)} \\ W_k U_{kk}^{(2)} \\ \vdots \\ W_k U_{kk}^{(l)} \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^{k-1} W_j U_{jk}^{(1)} \\ \sum_{j=1}^{k-1} W_j U_{jk}^{(2)} \\ \vdots \\ \sum_{j=1}^{k-1} W_j U_{jk}^{(l)} \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^k W_j U_{jk}^{(1)} \\ \sum_{j=1}^k W_j U_{jk}^{(2)} \\ \vdots \\ \sum_{j=1}^k W_j U_{jk}^{(l)} \end{bmatrix}. \end{aligned}$$

This is just the desired relation (4.3), and thus the proof of Theorem 3.1 is complete.

4.2 Proof of Theorem 3.2.

We proceed in the same fashion as in Subsection 4.1. Again, without loss of generality, we assume that the basis matrix \mathcal{V} in (3.10) is given by (4.1), and we partition the matrices W and $U^{(i)}$, $i = 1, 2, \dots, l$, as in (4.2). Inserting (4.1) and (4.2) into (3.10), it follows that the desired relation (3.10) holds true if, and only if,

$$(4.6) \quad \mathcal{M}^{k-1} \mathcal{R}_k = \begin{bmatrix} C^{(1)} \sum_{j=1}^k W_j U_{jk}^{(1)} \\ C^{(2)} \sum_{j=1}^k W_j U_{jk}^{(2)} \\ \vdots \\ C^{(l)} \sum_{j=1}^k W_j U_{jk}^{(l)} \end{bmatrix}, \quad k = 1, 2, \dots, k_0.$$

Therefore, it remains to construct the subblocks in (4.2) such that (4.6) is satisfied. To this end, we define these subblocks recursively as follows.

For $k = 1, 2, \dots, k_0$, we set

$$(4.7) \quad U_{jk}^{(i)} := \begin{cases} \sigma_i U_{j,k-1}^{(i)} E_k, & \text{for } j = 1, 2, \dots, k-1, \\ I_{m_k}, & \text{for } j = k, \end{cases}$$

for all $i = 1, 2, \dots, l$, and

$$(4.8) \quad W_k := \begin{cases} RE_1, & \text{if } k = 1, \\ \left(\sum_{i=1}^l M^{(i)} C^{(i)} \left(\sum_{j=1}^{k-1} W_j U_{j,k-1}^{(i)} \right) \right) E_k, & \text{if } k > 1. \end{cases}$$

Here, again, the matrices E_k are the ones from (2.4).

Using induction on k , we now show that the subblocks (4.7) and (4.8) indeed satisfy (4.6). Recall that \mathcal{R} is of form (3.8) and that, by (2.4) (for $k = 1$), $\mathcal{R}_1 = \mathcal{R}E_1$. Together with the definitions of $U_{11}^{(i)}$, $i = 1, 2, \dots, l$, in (4.7) and of W_1 in (4.8), it follows that

$$\mathcal{R}_1 = \begin{bmatrix} C^{(1)} \\ C^{(2)} \\ \vdots \\ C^{(l)} \end{bmatrix} (RE_1) = \begin{bmatrix} C^{(1)} W_1 U_{11}^{(1)} \\ C^{(2)} W_1 U_{11}^{(2)} \\ \vdots \\ C^{(l)} W_1 U_{11}^{(l)} \end{bmatrix}.$$

This is just (4.6) for $k = 1$. Let $1 < k \leq k_0$ and assume that (4.6) holds true for $k - 1$. Then, by multiplying the relation (4.6) (with k replaced by $k - 1$) from

the left by the matrix \mathcal{M} from (3.8), it follows that

$$\begin{aligned} \mathcal{M}^{k-1}\mathcal{R}_{k-1} &= \mathcal{M}\left(\mathcal{M}^{k-2}\mathcal{R}_{k-1}\right) \\ &= \begin{bmatrix} C^{(1)} \\ C^{(2)} \\ \vdots \\ C^{(l)} \end{bmatrix} \left(\sum_{i=1}^l M^{(i)} C^{(i)} \left(\sum_{j=1}^{k-1} W_j U_{j,k-1}^{(i)} \right) \right) + \begin{bmatrix} C^{(1)} \sum_{j=1}^{k-1} W_j \sigma_1 U_{j,k-1}^{(1)} \\ C^{(2)} \sum_{j=1}^{k-1} W_j \sigma_2 U_{j,k-1}^{(2)} \\ \vdots \\ C^{(l)} \sum_{j=1}^{k-1} W_j \sigma_l U_{j,k-1}^{(l)} \end{bmatrix}. \end{aligned}$$

Multiplying this relation from the right by the matrix E_k from (2.4) and using the definitions of $U_{jk}^{(i)}$, $i = 1, 2, \dots, l$, $j = 1, 2, \dots, k$, in (4.7) and of W_k in (4.8), we obtain

$$\begin{aligned} \mathcal{M}^{k-1}\mathcal{R}_k &= \mathcal{M}^{k-1}\mathcal{R}_{k-1}E_k \\ &= \begin{bmatrix} C^{(1)}W_k U_{kk}^{(1)} \\ C^{(2)}W_k U_{kk}^{(2)} \\ \vdots \\ C^{(l)}W_k U_{kk}^{(l)} \end{bmatrix} + \begin{bmatrix} C^{(1)} \sum_{j=1}^{k-1} W_j U_{jk}^{(1)} \\ C^{(2)} \sum_{j=1}^{k-1} W_j U_{jk}^{(2)} \\ \vdots \\ C^{(l)} \sum_{j=1}^{k-1} W_j U_{jk}^{(l)} \end{bmatrix} = \begin{bmatrix} C^{(1)} \sum_{j=1}^k W_j U_{jk}^{(1)} \\ C^{(2)} \sum_{j=1}^k W_j U_{jk}^{(2)} \\ \vdots \\ C^{(l)} \sum_{j=1}^k W_j U_{jk}^{(l)} \end{bmatrix}. \end{aligned}$$

This is just the desired relation (4.6), and thus the proof of Theorem 3.2 is complete.

5 Matrices arising in higher-order linear dynamical systems.

In this section, we show how block-Krylov subspaces $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$ with matrices \mathcal{M} and \mathcal{R} of the form (3.1) arise in the context of higher-order linear dynamical systems.

5.1 General time-invariant linear dynamical systems.

We consider general higher-order multi-input multi-output time-invariant linear dynamical systems. We denote by m and p the number of inputs and outputs, respectively, and by l the order of such systems. In the following, the only assumption on m , p , and l is that $m, p, l \geq 1$.

An m -input p -output time-invariant linear dynamical system of order l is a system of differential-algebraic equations (DAEs) of the following form:

$$\begin{aligned} (5.1) \quad P_l \frac{d^l}{dt^l} x(t) + P_{l-1} \frac{d^{l-1}}{dt^{l-1}} x(t) + \cdots + P_1 \frac{d}{dt} x(t) + P_0 x(t) &= Bu(t), \\ y(t) &= Du(t) + L_{l-1} \frac{d^{l-1}}{dt^{l-1}} x(t) + \cdots + L_1 \frac{d}{dt} x(t) + L_0 x(t). \end{aligned}$$

Here, $P_i \in \mathbb{C}^{n_0 \times n_0}$, $0 \leq i \leq l$, $B \in \mathbb{C}^{n_0 \times m}$, $D \in \mathbb{C}^{p \times m}$, and $L_j \in \mathbb{C}^{p \times n_0}$, $0 \leq j < l$, are given matrices, and n_0 is called the state-space dimension of (5.1).

Moreover, in (5.1), $u : [t_0, \infty) \mapsto \mathbb{C}^m$ is a given input function, $t_0 \in \mathbb{R}$ is a given initial time, the components of the vector-valued function $x : [t_0, \infty) \mapsto \mathbb{C}^{n_0}$ are the so-called state variables, and $y : [t_0, \infty) \mapsto \mathbb{C}^p$ is the output function. The system is completed by initial conditions of the form

$$(5.2) \quad \left. \frac{d^j}{dt^j} x(t) \right|_{t=t_0} = x_0^{(j)}, \quad 0 \leq j < l,$$

where $x_0^{(j)} \in \mathbb{C}^{n_0}$, $0 \leq j < l$, are given vectors.

We stress that the matrix P_l is allowed to be singular, and thus the first equation in (5.1) is indeed a system of DAEs in general. Our only assumption on the matrices P_i , $0 \leq i \leq l$, in (5.1) is that the $n_0 \times n_0$ -matrix-valued polynomial

$$(5.3) \quad P(s) := s^l P_l + s^{l-1} P_{l-1} + \cdots + s P_1 + P_0, \quad s \in \mathbb{C},$$

is *regular*, i.e., the matrix $P(s)$ is singular only for finitely many values of $s \in \mathbb{C}$; see, e.g., [12, Part II].

5.2 Equivalent first-order formulation.

It is well known (see, e.g., [12, Chapter 7]) that any l -th-order system (5.1) (with state-space dimension n_0) is equivalent to a first-order system with state-space dimension $N := ln_0$. Indeed, it is easy to verify that the l -th-order system (5.1) with initial conditions (5.2) is equivalent to the first-order system

$$(5.4) \quad \begin{aligned} \mathcal{E} \frac{d}{dt} z(t) - \mathcal{A} z(t) &= \mathcal{B} u(t), \\ y(t) &= \mathcal{D} u(t) + \mathcal{L} z(t), \\ z(t_0) &= z_0, \end{aligned}$$

where

$$z(t) := \begin{bmatrix} x(t) \\ \frac{d}{dt}x(t) \\ \vdots \\ \frac{d^{l-1}}{dt^{l-1}}x(t) \end{bmatrix}, \quad z_0 := \begin{bmatrix} x_0^{(0)} \\ x_0^{(1)} \\ \vdots \\ x_0^{(l-1)} \end{bmatrix},$$

$$(5.5) \quad \mathcal{L} := [L_0 \quad L_1 \quad \cdots \quad L_{l-1}], \quad \mathcal{B} := \begin{bmatrix} 0 \\ \vdots \\ 0 \\ B \end{bmatrix}, \quad \mathcal{D} := D,$$

$$\mathcal{E} := \begin{bmatrix} I & 0 & 0 & \cdots & 0 \\ 0 & I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & I & 0 \\ 0 & \cdots & 0 & 0 & P_l \end{bmatrix}, \quad \mathcal{A} := - \begin{bmatrix} 0 & -I & 0 & \cdots & 0 \\ 0 & 0 & -I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & -I \\ P_0 & P_1 & P_2 & \cdots & P_{l-1} \end{bmatrix},$$

and $I = I_{n_0}$ is the $n_0 \times n_0$ identity matrix.

It is easy to see that, for any given $s \in \mathbb{C}$, the matrix $s\mathcal{E} - \mathcal{A}$ is singular if, and only if, the matrix $P(s)$ defined in (5.3) is singular. Therefore, our assumption on the regularity of the matrix polynomial (5.3) is equivalent to the regularity of the matrix pencil $s\mathcal{E} - \mathcal{A}$. This guarantees that the matrix $s\mathcal{E} - \mathcal{A}$ is singular only for finitely many values of $s \in \mathbb{C}$, and that

$$(5.6) \quad H(s) := \mathcal{D} + \mathcal{L}(s\mathcal{E} - \mathcal{A})^{-1}\mathcal{B}, \quad s \in \mathbb{C},$$

is a well-defined $p \times m$ -matrix-valued rational function. We remark that (5.6) is called the frequency-domain *transfer function* of (5.4).

5.3 Padé-type model reduction.

A reduced-order model of (5.4) is a linear dynamical system of the same type as (5.4), but with reduced state-space dimension, say n , instead of the original state-space dimension N . More precisely, a *reduced-order model* of (5.4) with state-space dimension n is a system of the form

$$\mathcal{E}_n \frac{d}{dt} \tilde{z}(t) - \mathcal{A}_n \tilde{z}(t) = \mathcal{B}_n u(t),$$

$$(5.7) \quad \tilde{y}(t) = \mathcal{D}_n u(t) + \mathcal{L}_n \tilde{z}(t),$$

$$\tilde{z}(t_0) = \tilde{z}_0,$$

where $\mathcal{A}_n, \mathcal{E}_n \in \mathbb{C}^{n \times n}$, $\mathcal{B}_n \in \mathbb{C}^{n \times m}$, $\mathcal{D}_n \in \mathbb{C}^{p \times m}$, $\mathcal{L}_n \in \mathbb{C}^{p \times n}$, and $\tilde{z}_0 \in \mathbb{C}^n$. The problem of model reduction then is to construct data matrices $\mathcal{A}_n, \mathcal{E}_n, \mathcal{B}_n,$

\mathcal{D}_n , and \mathcal{L}_n such that (5.7) is a good approximation of the original system (5.4), even for $n \ll N$.

A possible approach, which is intimately related to block-Krylov subspaces, is Padé and Padé-type model reduction; see, e.g., [9, 11] and the references given there. Let $s_0 \in \mathbb{C}$ be a suitably chosen expansion point, and in particular, let s_0 be such that the matrix $s_0 \mathcal{E} - \mathcal{A}$ is nonsingular. The reduced system (5.7) is said to be an n -th Padé model of the original system (5.4) if the reduced-order transfer function

$$H_n(s) := \mathcal{D}_n + \mathcal{L}_n (s \mathcal{E}_n - \mathcal{A}_n)^{-1} \mathcal{B}_n, \quad s \in \mathbb{C},$$

and the original transfer function (5.6), H , agree in as many leading Taylor coefficients about the expansion point s_0 as possible, i.e.,

$$(5.8) \quad H_n(s) = H(s) + \mathcal{O}((s - s_0)^{q(n)}),$$

where $q(n)$ is as large as possible. While Padé models are optimal in the sense of (5.8), in general, they do not preserve other desirable properties of the original system. Preserving such properties is often possible by relaxing (5.8) to

$$(5.9) \quad H_n(s) = H(s) + \mathcal{O}((s - s_0)^{\hat{q}}),$$

where $\hat{q} < q(n)$. The reduced system (5.7) is said to be an n -th Padé-type model of the original system (5.4) if a property of the form (5.9) is satisfied.

Both n -th Padé and Padé-type models can be generated via Krylov-subspace machinery; see, e.g., [9, 11] and the references given there. To this end, the original transfer function (5.6) is rewritten in the form

$$H(s) = \mathcal{D} + \mathcal{L}(\mathcal{I} + (s - s_0)\mathcal{M})^{-1}\mathcal{R},$$

where

$$(5.10) \quad \mathcal{M} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{E} \quad \text{and} \quad \mathcal{R} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{B}.$$

Padé-type models are then obtained by projecting the data matrices in (5.4) onto the block-Krylov subspaces $\mathcal{K}_n(\mathcal{M}\mathcal{C}, \mathcal{R})$ induced by the matrices (5.10). Similarly, Padé models can be generated via two-sided projections involving the right and left block-Krylov subspaces $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$ and $\mathcal{K}_n(\mathcal{M}^H, \mathcal{L}^H)$.

5.4 Structure of the matrices \mathcal{M} and \mathcal{R} .

Recall that, in this section, we are concerned with general l -th-order systems of the form (5.1). In this case, the matrices \mathcal{A} , \mathcal{E} , and \mathcal{B} in (5.10) are the ones defined in (5.5). Furthermore, the expansion point $s_0 \in \mathbb{C}$ in (5.10) is such that the matrix $s_0 \mathcal{E} - \mathcal{A}$ is nonsingular, or, equivalently, the matrix

$$(5.11) \quad P(s_0) = s_0^l P_l + s_0^{l-1} P_{l-1} + \cdots + s_0 P_1 + P_0 \quad \text{is nonsingular.}$$

Next, we set

$$(5.12) \quad M^{(i)} := (P(s_0))^{-1} \sum_{j=0}^{l-i} s_0^j P_{i+j}, \quad i = 1, 2, \dots, l,$$

and

$$(5.13) \quad R := (P(s_0))^{-1}B.$$

Using the definitions of \mathcal{A} , \mathcal{E} , and \mathcal{B} in (5.10), together with (5.12) and (5.13), one can show that the matrices (5.10) have the representations

$$(5.14) \quad \mathcal{M} = \begin{bmatrix} M^{(1)} & M^{(2)} & M^{(3)} & \cdots & M^{(l)} \\ s_0 M^{(1)} & s_0 M^{(2)} & s_0 M^{(3)} & \cdots & s_0 M^{(l)} \\ s_0^2 M^{(1)} & s_0^2 M^{(2)} & s_0^2 M^{(3)} & \cdots & s_0^2 M^{(l)} \\ \vdots & \vdots & \vdots & & \vdots \\ s_0^{l-2} M^{(1)} & s_0^{l-2} M^{(2)} & s_0^{l-2} M^{(3)} & \cdots & s_0^{l-2} M^{(l)} \end{bmatrix}$$

$$- \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ I_{n_0} & 0 & \ddots & & \vdots \\ s_0 I_{n_0} & I_{n_0} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ s_0^{l-2} I_{n_0} & \cdots & s_0 I_{n_0} & I_{n_0} & 0 \end{bmatrix},$$

and

$$(5.15) \quad \mathcal{R} = \begin{bmatrix} I_{n_0} \\ s_0 I_{n_0} \\ s_0^2 I_{n_0} \\ \vdots \\ s_0^{l-1} I_{n_0} \end{bmatrix} R.$$

Proofs of (5.14) and (5.15) are given in Appendix A.

Note that the matrices \mathcal{M} and \mathcal{R} in (5.14) and (5.15) are a special instance of the class of matrices (3.1), with c and Σ given by

$$c := \begin{bmatrix} 1 \\ s_0 \\ s_0^2 \\ \vdots \\ s_0^{l-1} \end{bmatrix} \quad \text{and} \quad \Sigma := - \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ 1 & 0 & \ddots & & \vdots \\ s_0 & 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ s_0^{l-2} & \cdots & s_0 & 1 & 0 \end{bmatrix}.$$

Furthermore, provided that $s_0 \neq 0$, the assumption on c in (3.3) is satisfied. We remark that for the case $s_0 = 0$, \mathcal{M} reduces to a block companion matrix, and \mathcal{R} reduces to a multiple of the first block unit vector. We do not consider this case, which is fundamentally different from the case $s_0 \neq 0$, in this paper.

6 Matrices arising in first-order integro-DAEs.

An important special case of (5.1) is *second-order systems*, that is, $l = 2$ in (5.1). For example, second-order systems arise in structural dynamics [16, 5,

19], circuit analysis [20, Chapter 3], and computational electromagnetics [24]. However, in some of these applications, a more suitable formulation of such systems is as systems of first-order integro-differential-algebraic equations (integro-DAEs). For example, this is the case for passive systems such as RCL electrical circuits consisting of only resistors, capacitors, and inductors; see, e.g., [15, Chapter 1], [6, Chapter 2], and [10, 11]. In this section, we show how block-Krylov subspaces $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$ with matrices \mathcal{M} and \mathcal{R} of the form (3.8) arise in the context of such systems of first-order integro-DAEs.

6.1 Systems of first-order integro-DAEs.

We consider m -input p -output systems of first-order *integro-DAEs* of the following form:

$$(6.1) \quad \begin{aligned} P_1 \frac{d}{dt} x(t) + P_0 x(t) + P_{-1} \int_{t_0}^t x(\tau) d\tau &= Bu(t), \\ y(t) &= Du(t) + Lx(t), \\ x(t_0) &= x_0. \end{aligned}$$

Here, $P_{-1}, P_0, P_1 \in \mathbb{C}^{n_0 \times n_0}$, $B \in \mathbb{C}^{n_0 \times m}$, $D \in \mathbb{C}^{p \times m}$, and $L \in \mathbb{C}^{p \times n_0}$ are given matrices, $t_0 \in \mathbb{R}$ is a given initial time, and $x_0 \in \mathbb{C}^{n_0}$ is a given vector of initial values.

We stress that the matrix P_1 is allowed to be singular, and thus the first equation in (6.1) is indeed a system of integro-DAEs in general. Our only assumption on the matrices P_{-1}, P_0 , and P_1 in (6.1) is that the $n_0 \times n_0$ -matrix-valued rational function

$$Q(s) := sP_1 + P_0 + \frac{1}{s}P_{-1}, \quad s \in \mathbb{C},$$

is *regular*, i.e., the matrix $Q(s)$ is singular only for finitely many values of $s \in \mathbb{C}$.

In practical applications, the matrices P_0 and P_1 are usually sparse, while the matrix P_{-1} is not always sparse. However, in those cases where the matrix P_{-1} itself is dense, P_{-1} is given as a product of the form

$$(6.2) \quad P_{-1} = F_1 G F_2^H$$

or

$$(6.3) \quad P_{-1} = F_1 G^{-1} F_2^H, \quad \text{with nonsingular } G,$$

where $F_1, F_2 \in \mathbb{C}^{n_0 \times \hat{n}_0}$ and $G \in \mathbb{C}^{\hat{n}_0 \times \hat{n}_0}$ are sparse matrices. We stress that in the case (6.2), the matrix G is not required to be nonsingular. In particular, for any matrix $P_{-1} \in \mathbb{C}^{n_0 \times n_0}$, there is always the trivial factorization (6.2) with $F_1 = F_2 = I_{n_0}$ and $G = P_{-1}$. Therefore, in the following, we assume that the matrix P_{-1} in (6.1) is given by a product of the form (6.2) or (6.3).

6.2 Equivalent first-order formulations.

In analogy to the case of higher-order systems (5.1), any system of integro-DAEs of the form (6.1) is equivalent to a first-order system of the form (5.4). In this subsection, we present such equivalent first-order formulations.

We distinguish the two cases (6.2) and (6.3). First assume that P_{-1} is given by (6.2). In this case, we set

$$(6.4) \quad z_1(t) := x(t) \quad \text{and} \quad z_2(t) := F_2^H \int_{t_0}^t x(\tau) d\tau.$$

By (6.2) and (6.4), the first relation in (6.1) can be rewritten as follows:

$$(6.5) \quad P_1 z_1'(t) + P_0 z_1(t) + F_1 G z_2(t) = Bu(t).$$

Moreover, (6.4) implies that

$$(6.6) \quad z_2'(t) = F_2^H z_1(t).$$

It follows from (6.4)–(6.6) that the system of integro-DAEs (6.1) (with P_{-1} given by (6.2)) is equivalent to a first-order system (5.4) where

$$(6.7) \quad z(t) := \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix}, \quad z_0 := \begin{bmatrix} x_0 \\ 0 \end{bmatrix}, \quad \mathcal{L} := [L \quad 0], \quad \mathcal{B} := \begin{bmatrix} B \\ 0 \end{bmatrix},$$

$$\mathcal{D} := D, \quad \mathcal{A} := \begin{bmatrix} -P_0 & -F_1 G \\ F_2^H & 0 \end{bmatrix}, \quad \mathcal{E} := \begin{bmatrix} P_1 & 0 \\ 0 & I_{\hat{n}_0} \end{bmatrix}.$$

Next, we assume that P_{-1} is given by (6.3). In this case, we set

$$(6.8) \quad z_1(t) := x(t) \quad \text{and} \quad z_2(t) := G^{-1} F_2^H \int_{t_0}^t x(\tau) d\tau.$$

By (6.3) and (6.8), the first relation in (6.1) can be rewritten as follows:

$$(6.9) \quad P_1 z_1'(t) + P_0 z_1(t) + F_1 z_2(t) = Bu(t).$$

Moreover, (6.8) implies that

$$(6.10) \quad G z_2'(t) = F_2^H z_1(t).$$

It follows from (6.8)–(6.10) that the system of integro-DAEs (6.1) (with P_{-1} given by (6.3)) is equivalent to a first-order system (5.4) where

$$(6.11) \quad z(t) := \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix}, \quad z_0 := \begin{bmatrix} x_0 \\ 0 \end{bmatrix}, \quad \mathcal{L} := [L \quad 0], \quad \mathcal{B} := \begin{bmatrix} B \\ 0 \end{bmatrix},$$

$$\mathcal{D} := D, \quad \mathcal{A} := \begin{bmatrix} -P_0 & -F_1 \\ F_2^H & 0 \end{bmatrix}, \quad \mathcal{E} := \begin{bmatrix} P_1 & 0 \\ 0 & G \end{bmatrix}.$$

6.3 Padé and Padé-type model reduction.

Just as in Subsection 5.3, based on the equivalent first-order formulations defined in (6.7), respectively (6.11), one can again introduce the notion of Padé and Padé-type reduced-order models of systems of integro-DAEs (6.1). In this case, we assume that the expansion point $s_0 \in \mathbb{C}$ is chosen such that $s_0 \neq 0$ and the matrix

$$(6.12) \quad Q_0 := Q(s_0) = s_0 P_1 + P_0 + \frac{1}{s_0} P_{-1}$$

is nonsingular. One readily verifies that this condition is equivalent to the nonsingularity of the matrix $s_0 \mathcal{E} - \mathcal{A}$. The matrices that induce the relevant block-Krylov subspaces $\mathcal{K}_n(\mathcal{M}, \mathcal{R})$ for Padé and Padé-type model reduction are again given by

$$(6.13) \quad \mathcal{M} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{E} \quad \text{and} \quad \mathcal{R} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{B},$$

where \mathcal{A} , \mathcal{E} , and \mathcal{B} are now the matrices defined in (6.7), respectively (6.11).

6.4 Structure of the matrices \mathcal{M} and \mathcal{R} .

In this subsection, we describe the structure of the matrices \mathcal{M} and \mathcal{R} .

Again, we distinguish the two cases (6.2) and (6.3). First assume that P_{-1} is given by (6.2). Using the definitions of \mathcal{A} , \mathcal{E} , \mathcal{B} in (6.7), and of Q_0 in (6.12), one can show that the matrices (6.13) have the representations

$$(6.14) \quad \begin{aligned} \mathcal{M} &= \begin{bmatrix} I_{n_0} \\ \frac{1}{s_0} F_2^H \end{bmatrix} \left[Q_0^{-1} P_1 \quad -\frac{1}{s_0} Q_0^{-1} F_1 G \right] + \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{s_0} I_{\hat{n}_0} \end{bmatrix}, \\ \mathcal{R} &= \begin{bmatrix} I_{n_0} \\ \frac{1}{s_0} F_2^H \end{bmatrix} Q_0^{-1} B. \end{aligned}$$

The matrices \mathcal{M} and \mathcal{R} in (6.14) are a special instance of the class of matrices (3.8), with the integers and matrices (3.9) chosen as follows:

$$\begin{aligned} l &:= 2, \quad n_1 := n_0, \quad n_2 := \hat{n}_0, \\ C^{(1)} &:= I_{n_0}, \quad C^{(2)} := \frac{1}{s_0} F_2^H, \\ M^{(1)} &:= Q_0^{-1} P_1, \quad M^{(2)} := -\frac{1}{s_0} Q_0^{-1} F_1 G, \\ \sigma_1 &:= 0, \quad \sigma_2 := \frac{1}{s_0}, \quad R := Q_0^{-1} B. \end{aligned}$$

Next, we assume that P_{-1} is given by (6.3). Using the definitions of \mathcal{A} , \mathcal{E} , \mathcal{B} in (6.11), and of Q_0 in (6.12), one can show that the matrices (6.13) have the representations

$$(6.15) \quad \begin{aligned} \mathcal{M} &= \begin{bmatrix} I_{n_0} \\ \frac{1}{s_0} G^{-1} F_2^H \end{bmatrix} \left[Q_0^{-1} P_1 \quad -\frac{1}{s_0} Q_0^{-1} F_1 \right] + \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{s_0} I_{\hat{n}_0} \end{bmatrix}, \\ \mathcal{R} &= \begin{bmatrix} I_{n_0} \\ \frac{1}{s_0} G^{-1} F_2^H \end{bmatrix} Q_0^{-1} B. \end{aligned}$$

Note that the matrices \mathcal{M} and \mathcal{R} in (6.15) are a special instance of the class of matrices (3.8), with the integers and matrices (3.9) chosen as follows:

$$\begin{aligned} l &:= 2, & n_1 &:= n_0, & n_2 &:= \hat{n}_0, \\ C^{(1)} &:= I_{n_0}, & C^{(2)} &:= \frac{1}{s_0} G^{-1} F_2^H, \\ M^{(1)} &:= Q_0^{-1} P_1, & M^{(2)} &:= -\frac{1}{s_0} Q_0^{-1} F_1, \\ \sigma_1 &:= 0, & \sigma_2 &:= \frac{1}{s_0}, & R &:= Q_0^{-1} B. \end{aligned}$$

Proofs of (6.14) and (6.15) are given in Appendix B.

7 Concluding remarks.

We have introduced two classes of structured matrices, which include the matrices of first-order formulations of higher-order linear dynamical systems as special cases. As our main results, we have shown that the block-Krylov subspaces induced by the matrices in these classes exhibit special structures. Roughly speaking, for both classes, the associated structured block-Krylov subspaces consist of multiple copies of certain subspaces of the state space of the original higher-order system. Note that the dimension of the state space of the first-order formulation is l times the dimension of the original l -th-order system. Our results show that in order to construct basis vectors for the block-Krylov subspaces of the higher-dimensional first-order state-space, it is sufficient to construct basis vectors for certain subspaces of the lower-dimensional l -th-order state space. The problem of the efficient and numerically stable construction of basis vectors of these subspaces is beyond the scope of this paper. Such algorithms will be described in a forthcoming report.

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Appendix A.

In this appendix, we establish the representations (5.14) and (5.15). To this end, we set

$$(7.1) \quad \hat{P}_i := \sum_{j=0}^{l-i} s_0^j P_{i+j}, \quad i = 0, 1, \dots, l.$$

In view of (5.11) and (5.12), we then have

$$(7.2) \quad M^{(i)} := \hat{P}_0^{-1} \hat{P}_i, \quad i = 1, 2, \dots, l, \quad \text{and} \quad \hat{P}_0 = P(s_0).$$

Using the definitions of \mathcal{A} and \mathcal{E} in (5.5), as well as (7.1), one readily verifies that

$$(7.3) \quad s_0 \mathcal{E} - \mathcal{A} = \begin{bmatrix} s_0 I & -I & 0 & \cdots & 0 \\ 0 & s_0 I & -I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & s_0 I & -I \\ P_0 & P_1 & \cdots & P_{l-2} & P_{l-1} + s_0 P_l \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -I & 0 & \cdots & 0 \\ 0 & 0 & -I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & -I \\ \hat{P}_0 & \hat{P}_1 & \hat{P}_2 & \cdots & \hat{P}_{l-1} \end{bmatrix} \begin{bmatrix} I & 0 & 0 & \cdots & 0 \\ -s_0 I & I & 0 & \cdots & 0 \\ 0 & -s_0 I & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -s_0 I & I \end{bmatrix}.$$

Note that, in view of (7.2), we have

$$\begin{bmatrix} 0 & -I & 0 & \cdots & 0 \\ 0 & 0 & -I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & -I \\ \hat{P}_0 & \hat{P}_1 & \hat{P}_2 & \cdots & \hat{P}_{l-1} \end{bmatrix}^{-1} = \begin{bmatrix} M^{(1)} & M^{(2)} & \cdots & M^{(l-1)} & \hat{P}_0^{-1} \\ -I & 0 & 0 & \cdots & 0 \\ 0 & -I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -I & 0 \end{bmatrix}.$$

By inverting the two factors on the right-hand side of (7.3) and multiplying the inverse factors (in reverse order) from the right by the matrix \mathcal{E} , respectively \mathcal{B} , from (5.5), we obtain the relation

$$\mathcal{M} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{E}$$

$$= \begin{bmatrix} I & 0 & \cdots & \cdots & 0 \\ s_0 I & I & 0 & \cdots & 0 \\ s_0^2 I & s_0 I & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ s_0^{l-1} I & \cdots & s_0^2 I & s_0 I & I \end{bmatrix} \begin{bmatrix} M^{(1)} & M^{(2)} & M^{(3)} & \cdots & M^{(l)} \\ -I & 0 & 0 & \cdots & 0 \\ 0 & -I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -I & 0 \end{bmatrix},$$

respectively

$$\mathcal{R} := (s_0 \mathcal{E} - \mathcal{A})^{-1} \mathcal{B} = \begin{bmatrix} I \\ s_0 I \\ s_0^2 I \\ \vdots \\ s_0^{l-1} I \end{bmatrix} (P(s_0))^{-1} B.$$

The first relation is readily rewritten in the form (5.14), and the second relation is just (5.15). Thus the proof is complete.

Appendix B.

In this appendix, we establish the representations (6.14) and (6.15) for the case that P_{-1} is of the form (6.2) and (6.3), respectively.

First assume that P_{-1} is given by (6.2). Using (6.2), (6.7), and (6.12), one readily verifies that

$$\begin{aligned} s_0 \mathcal{E} - \mathcal{A} &= \begin{bmatrix} s_0 P_1 + P_0 & F_1 G \\ -F_2^H & s_0 I_{\hat{n}_0} \end{bmatrix} \\ &= \begin{bmatrix} Q_0 & F_1 G \\ 0 & s_0 I_{\hat{n}_0} \end{bmatrix} \begin{bmatrix} I_{n_0} & 0 \\ -\frac{1}{s_0} F_2^H & I_{\hat{n}_0} \end{bmatrix}. \end{aligned}$$

It follows that

$$(7.4) \quad (s_0 \mathcal{E} - \mathcal{A})^{-1} = \begin{bmatrix} I_{n_0} & 0 \\ \frac{1}{s_0} F_2^H & I_{\hat{n}_0} \end{bmatrix} \begin{bmatrix} Q_0^{-1} & -\frac{1}{s_0} Q_0^{-1} F_1 G \\ 0 & \frac{1}{s_0} I_{\hat{n}_0} \end{bmatrix}.$$

By multiplying (7.4) from the right by the matrix \mathcal{E} , respectively \mathcal{R} , from (6.7), we obtain the relations stated in (6.14).

Next, we assume that P_{-1} is given by (6.3). Recall that the matrix G is nonsingular. In this case, we have

$$\begin{aligned} s_0 \mathcal{E} - \mathcal{A} &= \begin{bmatrix} s_0 P_1 + P_0 & F_1 \\ -F_2^H & s_0 G \end{bmatrix} \\ &= \begin{bmatrix} Q_0 & F_1 \\ 0 & s_0 G \end{bmatrix} \begin{bmatrix} I_{n_0} & 0 \\ -\frac{1}{s_0} G^{-1} F_2^H & I_{\hat{n}_0} \end{bmatrix}. \end{aligned}$$

It follows that

$$(7.5) \quad (s_0 \mathcal{E} - \mathcal{A})^{-1} = \begin{bmatrix} I_{n_0} & 0 \\ \frac{1}{s_0} G^{-1} F_2^H & I_{\hat{n}_0} \end{bmatrix} \begin{bmatrix} Q_0^{-1} & -\frac{1}{s_0} Q_0^{-1} F_1 G^{-1} \\ 0 & \frac{1}{s_0} G^{-1} \end{bmatrix}.$$

By multiplying (7.5) from the right by the matrix \mathcal{E} , respectively \mathcal{R} , from (6.7), we obtain the relations stated in (6.15).