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MOMENT MATCHING THEOREMS FOR DIMENSION REDUCTION OF HIGHER-ORDER DYNAMICAL SYSTEMS VIA HIGHER-ORDER KRYLOV SUBSPACES *

TSUYOSHI KOYAMA† AND SANJAY GOVINDJEE †

Abstract. Moment matching theorems for Krylov subspace based model reduction of higher-order linear dynamical systems are presented in the context of higher-order Krylov subspaces. We introduce the definition of a *nth-order Krylov subspace* $\mathcal{K}^n_k(\{\mathbf{A}_i\}^n_{i=1};\mathbf{u})$ based on a sequence of n square matrices $\{\mathbf{A}_i\}^n_{i=1}$ and vector $\mathbf{u}$. This subspace is a generalization of Krylov subspaces for higher-order systems, incorporating the standard Krylov subspace $\mathcal{K}_k(\mathbf{A};\mathbf{u})$ and the second-order Krylov subspace $\mathcal{G}_k(\mathbf{A},\mathbf{B};\mathbf{u})$ as special cases. Krylov subspace based structure preserving model reduction onto this subspace eliminates the linearization step of rewriting the higher-order system in an equivalent first-order form to prove moment-matching properties.

Key words. model reduction, moment matching, second-order Krylov subspace, higher-order Krylov subspaces

AMS subject classification. 65F99

1. Introduction.

Linear dynamical systems of order two and higher appear in the modeling of many physical settings such as electromagnetic, mechanical, and thermal systems as well as systems coupling any number of these physical domains. In many applications, these systems are excited by a single-input and a single-output. The numerical discretization of such systems results in a continuous time-invariant single-input single-output (SISO) model described by,

$$\begin{aligned}\sum_{i=0}^{n}\mathbf{D}_i\frac{d^i}{dt^i}\mathbf{x}(t) &= \mathbf{b}u(t)\ ,\\ y(t) &= \mathbf{l}^*\mathbf{x}(t)\ ,\end{aligned}\tag{1.1}$$

with initial conditions, $\frac{d^i}{dt^i}\mathbf{x}(0)=\mathbf{x}_0^{(i)}$, $i=0,\dots,n$. Here t is the time variable, n is the order of the differential equation, $\mathbf{x}(t)\in\mathbb{C}^N$ is a complex valued state vector, and N is the state space dimension. $u(t)$ is the scalar valued input function and $y(t)$ is the scalar valued output function. $\{\mathbf{D}_i\in\mathbb{C}^{N\times N}\}^n_{i=0}$ are the coefficient matrices and $\mathbf{b},\mathbf{l}\in\mathbb{C}^N$ are the vectors which define the input and output distribution. This SISO system is characterized by its transfer function,

$$H(s)=\mathbf{l}^*\left(\sum_{i=0}^{n}s^i\mathbf{D}_i\right)^{-1}\mathbf{b}\ .\tag{1.2}$$

Treatment of the system (1.1) and its corresponding transfer function (1.2) can be computationally challenging when the size of the state space N is on the order of millions or larger. Spatial numerical discretization of time-dependent partial differential equations arising from continuum systems is an example of such a case. To reduce the time and computational effort for evaluation of these systems, reduced-order modeling techniques which can preserve the characteristics of the original system with a substantially smaller size state space $N_R \ll N$ are desired.

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Krylov subspace based model reduction of linear dynamical systems has grown in popularity due to its generality and computational efficiency in applications to large-scale systems [1, 5]. This technique is generally categorized as a member of the family of moment-matching methods [2]. The standard approach of Krylov subspace based model reduction methods for a higher-order linear dynamical system (1.1,1.2) is to perform a mathematically equivalent linearization to a first-order system by introduction of auxiliary variables, followed by application of standard Krylov subspace techniques for first-order systems. This approach has two disadvantages. The first is the increase in the size of the system one must manipulate. In a nth-order system with state space of size N, the equivalent first-order system involves a state space of size nN, increasing the computational costs. The second is the lack of preservation of the structure of the original system in the reduced-order model; neither the physical character of the coefficient matrices of the original nth-order system nor its nth-order structure is preserved.

To remedy these disadvantages in the case of second-order systems, techniques treating the second-order system in its original form have been developed; see e.g.the pioneering work by Su and Craig [12]. Bai and Su [3, 4] as well as Salimbahrami and Lohmann [10] define a second-order Krylov subspace $\mathcal{G}_k(\mathbf{A}, \mathbf{B}; \mathbf{u})$ and prove that model reduction using this subspace yields desired moment matching properties. Bai and Su also observe that the standard Krylov subspace generated by a specific choice of an equivalent first-order system contains "two copies" of the second-order Krylov subspace. This correspondence between the original second-order system and the equivalent first-order system is exploited in the proof of the moment matching theorem presented for the equivalent first-order system. Further, these authors clearly identify that the relevant subspace for structure preserving model reduction of the second-order system is the second-order Krylov subspace. The second-order Krylov subspace is also shown to outperform the standard Krylov subspace in terms of a projection space for the quadratic eigenvalue problem arising from second-order systems [4]. The work of Li and Bai [8] focuses on the concept of structure preserving model reduction, presenting a more general moment-matching theorem for first-order systems invoking projectors. The structure of the equivalent first-order system obtained from the second-order system is exploited to prove the moment matching properties similar to Bai and Su [3].

For the case of higher-order systems, a Krylov subspace based model reduction method which directly treats the system in its original form are rare. To the best of the authors knowledge, the work by Slone [11] presenting a method in the context of asymptotic waveform evaluation (AWE) techniques, is the only one in existence. In this method, a sequence of vectors which coincide with the sequence of vectors spanning the right-like nth order Krylov subspace that we present is constructed and used to construct the reduced-order model. Since the method is based strictly on this single sequence as well as considering only projections with the same subspace from the left and right, it lacks the flexibility of matching more moments by oblique projections as well as incorporating a union of subspaces for moment-matching at multiple expansion points.

As mentioned earlier, the standard technique is to rewrite the nth-order system as an equivalent first-order system and employ standard Krylov subspace techniques for model reduction of first-order systems. Freund [6] has proven that the standard Krylov subspace generated from the equivalent first-order system of size nN for an nth-order system contains "multiple copies" of the same subspace. We remark here that the case proven by Freund differs from the claim made by Li and Bai [3] for the second-order system, such that the standard Krylov subspace generated by the equivalent first-order system contains "two copies" of the second-order Krylov subspace. Freund has taken the shift-"after"-linearization approach in the case of constructing approximations near a point $s_0 \neq 0$. This approach generates a different standard Krylov subspace from the shift-"before"-linearization approach taken by Li and Bai. The two cases are identical in the case $s_0 = 0$. Li and Bai make a remark in their paper that their theorem is directly applicable to higher-order systems, but we find this to be not necessarily true.

In this paper, higher-order systems are treated without a transformation to an equivalent first-order system. The presented results extend the work of Li and Bai [8] and Bai and Su [3]. The nth-order Krylov subspace, a generalization of Krylov subspaces, is introduced. In the case of $n = 1$, however, it reduces to the standard Krylov subspace, and in the case of $n = 2$, it reduces to the second-order Krylov subspace. A moment matching theorem for higher-order systems is then presented, where the projection subspaces are enforced to contain nth-order Krylov subspaces. The projection subspaces can contain nth-order Krylov subspaces at multiple expansion points for multipoint moment-matching, a feature lacking in the method by Slone [11]. Compared to the theorem presented by Li and Bai, our theorem requires no conversion to an equivalent first-order system to prove the moment matching property of higher-order systems, enabling ease in application and removal of auxiliary variables and matrices. Connections are also made between the nth-order Krylov subspace and the standard Krylov subspace generated from the equivalent first-order system under a shift-"before"-linearization approach.

The remainder of the paper is organized as follows. In Section 2, the definition of moments of the transfer function and its representation in terms of the coefficient matrices of the transfer function is introduced. This representation motivates the definition of the nth-order Krylov subspace introduced in Section 3. In Section 4, the moment matching theorems utilizing projectors are presented along with several lemmas required to prove the theorem. In Section 5, the connection between the nth-order Krylov subspace and the standard Krylov subspace generated from the equivalent first-order system under a shift-"before"-linearization approach is presented. This correspondence shows the equivalence of the two subspaces.

Throughout this paper, $\mathbb{C}$, $\mathbb{C}^N$, and $\mathbb{C}^{M\times N}$ are the sets of complex numbers, column vectors of dimension N, and $M \times N$ complex matrices, respectively. Boldface letters are used to denote vectors (lower cases) and matrices (upper cases), and $\mathbf{I}$ for the identity matrix. $(\cdot)^*$ denotes the complex conjugate transpose, $(\cdot)^T$ denotes the transpose, and $(\cdot)^{-*} = (\cdot^*)^{-1}$ denotes the complex conjugate transpose inverse. $\mathsf{span}(\mathbf{X})$ denotes the space spanned by the columns of the matrix $\mathbf{X}$, and $\mathsf{span}\{\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_{k-1}\}$ denotes the space spanned by the vector sequence $\{\mathbf{r}_i\}_{i=0}^{k-1}$.

2. Moments of the transfer function. In this section, the definition of the moments of a transfer function are reviewed and expressions for the moments are presented.

The transfer function is obtained by taking the Laplace transform of system (1.1),

$$\begin{aligned} \sum_{i=0}^{n} s^i \mathbf{D}_i \widetilde{\mathbf{x}}(s) &= \mathbf{b}\widetilde{u}(s) \ , \\ \widetilde{y}(s) &= \mathbf{l}^* \widetilde{\mathbf{x}}(s) \ , \end{aligned} \tag{2.1}$$

where the tilde's represent the Laplace transform of each variable. For simplicity we have assumed zero initial conditions, $\frac{d^i}{dt^i}\mathbf{x}(0) = \mathbf{0}$, $i = 0, \dots, n$. Eliminating $\widetilde{\mathbf{x}}(s)$ in (2.1) results in the equation $\widetilde{y}(s) = H(s)\widetilde{u}(s)$, where $H(s)$ is the scalar valued SISO system transfer function:

$$H(s) = \mathbf{l}^* \left(\sum_{i=0}^{n} s^i \mathbf{D}_i \right)^{-1} \mathbf{b} \ . \tag{2.2}$$

The moments of a function are defined as the coefficients of the power series expansion around a given point. The transfer function expanded at $s = 0$ is,

$$H(s) = \sum_{i=0}^{\infty} M_i s^i \ , \tag{2.3}$$

where M_i are the moments. We present the following lemma to compute the moments of the nth-order system.

LEMMA 2.1. *A function of the form,*

$$f(s) = \mathbf{p}^* \left(\mathbf{I} - \sum_{i=1}^{n} s^i \mathbf{A}^i \ , \right)^{-1} \mathbf{q} \tag{2.4}$$

has the representation around $s = 0$,

$$f(s) = \sum_{i=0}^{\infty} \left(\mathbf{p}^* \mathbf{E}^i \mathbf{q} \right) s^i \ , \tag{2.5}$$

where $\mathbf{A}^i \in \mathbb{C}^{N \times N}$, $1 \leq i \leq n$ are given matrices, and $\mathbf{p},\ \mathbf{q} \in \mathbb{C}^N$ are given vectors. The sequence of matrices $\mathbf{E}^k \in \mathbb{C}^{N \times N}$ $(0 \leq k)$ are given by the recursion,

$$\begin{aligned} \mathbf{E}^0 &= \mathbf{I} \ , \\ \mathbf{E}^k &= \sum_{i=1}^{min(k,n)} \mathbf{A}^i \ \mathbf{E}^{k-i} = \sum_{i=1}^{min(k,n)} \mathbf{E}^{k-i} \ \mathbf{A}^i \qquad (1 \leq k) \ . \end{aligned} \tag{2.6}$$

Proof. The proof of this Lemma follows as a consequence of Lemma A.1 in the Appendix. □

Using Lemma 2.1 and the assumption that $\mathbf{D}_0$ is invertible, (2.2) can be written in the following two equivalent forms,

$$\begin{aligned} H(s) &= \mathbf{l}^* \left(\mathbf{I} + \sum_{i=1}^{n} s^i \mathbf{D}_0^{-1} \mathbf{D}_i \right)^{-1} \mathbf{D}_0^{-1} \mathbf{b} \\ &= \sum_{i=0}^{\infty} \left[\mathbf{l}^* \mathbf{E}_r^i \left(\mathbf{D}_0^{-1} \mathbf{b} \right) \right] s^i \ , \end{aligned} \tag{2.7}$$

where $\{\mathbf{E}_r^i\}_{i=0}^{\infty}$ is defined by the recursion in Lemma 2.1 with the substitution of $\mathbf{A}_r^i$ for $\mathbf{A}^i$, where

$$\mathbf{A}_r^i = -\mathbf{D}_0^{-1} \mathbf{D}_i, \quad (1 \leq i \leq n) \ , \tag{2.8}$$

or equivalently,

$$
\begin{aligned}
H(s) &= \mathbf{l}^* \mathbf{D}_0^{-1} \left(\mathbf{I} + \sum_{i=1}^{n} s^i \mathbf{D}_i \mathbf{D}_0^{-1} \right)^{-1} \mathbf{b} \\
&= \left[\mathbf{b}^* \left(\mathbf{I} + \sum_{i=1}^{n} s^{*i} \mathbf{D}_0^{-*} \mathbf{D}_i^* \right)^{-1} \mathbf{D}_0^{-*} \mathbf{l} \right]^* \\
&= \sum_{i=0}^{\infty} \left[\mathbf{b}^* \mathbf{E}_l^i \left(\mathbf{D}_0^{-*} \mathbf{l} \right) \right]^* s^i \quad , \qquad (2.9)
\end{aligned}
$$

where, $\{\mathbf{E}_l^i\}_{i=0}^{\infty}$ is defined by the recursion in Lemma 2.1 with the substitution of $\mathbf{A}_l^i$ for $\mathbf{A}^i$, where

$$\mathbf{A}_l^i = -\mathbf{D}_0^{-*} \mathbf{D}_i^*, \quad (1 \le i \le n) \ . \qquad (2.10)$$

The two forms are presented here to motivate the construction of the projection subspaces selected in Section 4 for model reduction. The subscripts for the sequences of matrices $\{\mathbf{E}_{(\cdot)}^i\}_{i=0}^{\infty}$ adhere to the convention, that r denotes the sequence generated by the right-like nth-order Krylov subspace and l denotes that generated by the left-like nth-order Krylov subspace in the sense that they are constructed using matrices that are conjugate transposes of each other. The expressions for the moments in the two cases are trivially identified as:

$$M_i = \mathbf{l}^* \mathbf{E}_r^i \mathbf{D}_0^{-1} \mathbf{b} = \mathbf{l}^* \mathbf{D}_0^{-1} \mathbf{E}_l^{i*} \mathbf{b} \ . \qquad (2.11)$$

The central goal of model reduction is to construct a model with less state space degrees of freedom than the original system while retaining desired properties of the original system, such as the structure of the coefficient matrices of the system $\{\mathbf{D}_i\}_{i=0}^{n}$, the order n of the system, and accuracy of the reduced order system transfer function as measured normally by the degree of moment matching. Let us define the reduced-order model system as:

$$
\begin{aligned}
\sum_{i=0}^{n} \mathbf{D}_{R,i} \frac{d^i}{dt^i} \mathbf{z}(t) &= \mathbf{b}_R u(t) \ , \\
y_R(t) &= \mathbf{l}_R^* \mathbf{z}(t) \ .
\end{aligned} \qquad (2.12)
$$

Here $\mathbf{z}(t) \in \mathbb{C}^{N_R}$ is the complex valued state vector, and $N_R \ll N$ is the state space dimension. $\{\mathbf{D}_{R,i} \in \mathbb{C}^{N_R \times N_R}\}_{i=0}^{n}$ are the coefficient matrices and $\mathbf{b}_R, \mathbf{l}_R \in \mathbb{C}^{N_R}$ are the vectors which define the input and output distribution. $y_R(t)$ is the scalar-valued output function of the reduced-order model. The corresponding transfer function $H_R(s)$ of this system is:

$$H_R(s) = \mathbf{l}_R^* \left(\sum_{i=0}^{n} s^i \mathbf{D}_{R,i} \right)^{-1} \mathbf{b}_R \ . \qquad (2.13)$$

By constructing a reduced-order model of the form (2.12), we can preserve the order of the system. The power series expansion of the transfer function (2.13) at $s = 0$ is,

$$H_R(s) = \sum_{i=0}^{\infty} M_{R,i} s^i \ , \qquad (2.14)$$

where $M_{R,i}$ are the moments. Following the same procedure for derivation of the moments of the full system, the reduced-order system moments are obtained as,

$$M_{R,i} = \mathbf{l}_R^* \mathbf{E}_{R,r}^i \mathbf{D}_{R,0}^{-1} \mathbf{b}_R = \mathbf{l}_R^* \mathbf{D}_{R,0}^{-1} \mathbf{E}_{R,l}^{i*} \mathbf{b}_R \quad , \tag{2.15}$$

where $\{\mathbf{E}_{R,r}^i\}_{i=0}^{\infty}$ is defined by the recursion in Lemma 2.1 with substitution of $\mathbf{A}_{R,r}^i$ for $\mathbf{A}^i$, where

$$\mathbf{A}_{R,r}^i = -\mathbf{D}_{R,0}^{-1} \mathbf{D}_{R,i}, \quad (1 \leq i \leq n) \ , \tag{2.16}$$

and, $\{\mathbf{E}_{R,l}^i\}_{i=0}^{\infty}$ is defined by the recursion in Lemma 2.1 with substitution of $\mathbf{A}_{R,l}^i$ for $\mathbf{A}^i$, where

$$\mathbf{A}_{R,l}^i = -\mathbf{D}_{R,0}^{-*} \mathbf{D}_{R,i}^*, \quad (1 \leq i \leq n) \ . \tag{2.17}$$

For accuracy, we desire that the moments of the transfer function of the reduced system, $M_{R,i}$, match those of the original system, M_i, for the largest q possible,

$$M_i = M_{R,i} \quad \text{for } i = 0, \ldots, q-1 \ . \tag{2.18}$$

This implies that $H_R(s)$ is a qth-order Padé approximant of $H(s)$:

$$H(s) = H_R(s) + O(s^q) \ . \tag{2.19}$$

The method we will employ to construct the reduced-order model (2.12) is based on subspace projection methods which are introduced in Section 4. We will see that these projections are intimately related to higher-order Krylov subspaces as will be introduced in Section 3.

REMARK 2.1 Though our results are presented for SISO systems, they generalize to multiple-input multiple-output (MIMO) systems. Consider the matrix-valued transfer function of a MIMO system,

$$\mathbf{H}(s) = \mathbf{L}^* \left(\sum_{i=0}^{n} s^i \mathbf{D}_i \right)^{-1} \mathbf{B} \ .$$

Here $\mathbf{B}, \mathbf{L} \in \mathbb{C}^{N \times p}$ for some p, are the matrices representing the input and output distributions. The matrix-valued moments of this transfer function are defined analogously as,

$$\mathbf{M}_i = \mathbf{L}^* \mathbf{E}_r^i \mathbf{D}_0^{-1} \mathbf{B} = \mathbf{L}^* \mathbf{D}_0^{-1} \mathbf{E}_l^{i\,*} \mathbf{B} \quad . \tag{2.20}$$

3. Higher-order Krylov subspaces. In this section, the definition of an nth-order Krylov subspace is introduced. This definition is a generalization of the kth standard Krylov subspace defined as,

$$\mathcal{K}_k(\mathbf{A}; \mathbf{u}) = \mathsf{span} \left\{ \mathbf{u}, \mathbf{A}\mathbf{u}, \ldots, \underbrace{\mathbf{A}\mathbf{A} \cdots \mathbf{A}}_{k-1}\mathbf{u} \right\} \ , \tag{3.1}$$

where $\mathbf{A} \in \mathbb{C}^{N\times N}$ and $\mathbf{u} \in \mathbb{C}^N$. A connection between the following sequence of matrices $\{\mathbf{E}^i\}_{i=0}^{\infty}$ defined in Lemma 2.1 and the kth nth-order Krylov subspace can be obtained by defining the following sequence and its span:

DEFINITION 3.1. *Let $\mathbf{A}^i \in \mathbb{C}^{N\times N}, 1 \le i \le n$ be given matrices, and let $\mathbf{u} \in \mathbb{C}^N$ be a nonzero vector. Let k also be given. Then the sequence*

$$\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_{k-1},$$

where

$$\begin{aligned} \mathbf{r}_0 &= \mathbf{u}\ , \\ \mathbf{r}_l &= \sum_{i=1}^{min(l,n)} \mathbf{A}^i \mathbf{r}_{l-i} \quad (1 \le l \le k-1)\ , \end{aligned} \tag{3.2}$$

is called the kth nth-order Krylov sequence based on $\{\mathbf{A}^i\}_{i=1}^n$ and $\mathbf{u}$. The space,

$$\mathcal{K}_k^n\left(\{\mathbf{A}^i\}_{i=1}^n; \mathbf{u}\right) = \mathsf{span}\left\{\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_{k-1}\right\}$$

is called a kth nth-order Krylov subspace.

The connection with the standard Krylov subspace $\mathcal{K}_k(\mathbf{A}; \mathbf{u})$ and second-order Krylov subspace $\mathcal{G}_k(\mathbf{A}, \mathbf{B}; \mathbf{u})$ is clear from this definition,

$$\begin{aligned} \mathcal{K}_k(\mathbf{A}; \mathbf{u}) &= \mathcal{K}_k^1(\mathbf{A}; \mathbf{u}) \quad \text{for } n = 1, \\ \mathcal{G}_k(\mathbf{A}, \mathbf{B}; \mathbf{u}) &= \mathcal{K}_k^2(\mathbf{A}, \mathbf{B}; \mathbf{u}) \quad \text{for } n = 2. \end{aligned}$$

Comparison between the definition of the nth-order Krylov subspace and the recursive nature of the sequence of matrices $\{\mathbf{E}^i\}_{i=0}^{\infty}$ in Lemma 2.1 reveals the following correspondence between this matrix sequence and sequence of vectors spanning the subspace.

LEMMA 3.2. *The sequence of vectors $\{\mathbf{r}_i\}_{i=0}^{k-1}$ spanning the kth nth-order Krylov subspace $\mathcal{K}_k^n\left(\{\mathbf{A}^i\}_{i=1}^n; \mathbf{u}\right)$ is defined by,*

$$\mathbf{r}_i = \mathbf{E}^i \mathbf{u}\ , \tag{3.3}$$

where $\{\mathbf{E}^i\}_{i=0}^{k-1}$ is the sequence of matrices defined in Lemma 2.1.
Proof. This is easily seen by comparing the expressions for $\mathbf{E}^i$ in Lemma 2.1 with that obtained from inserting (3.3) into (3.2). ∎

REMARK 3.1 One can easily construct a numerical algorithm to generate an orthogonal basis spanning a nth-order Krylov subspace similar to the Second Order Arnoldi (SOAR) method [4] for second-order systems. One algorithm by the name of well-conditioned asymptotic waveform evaluation (WCAWE) [11] for constructing a non-orthogonal subspace exists, though the constructed subspace is not identified as a generalization of the standard Krylov subspace.

REMARK 3.2 The definition of the kth nth-order Krylov subspace also naturally generalizes to block-Krylov subspaces of the form, $\mathcal{K}_k^n\left(\{\mathbf{A}^i\}_{i=1}^n; \mathbf{U}\right)$, where $\mathbf{U} \in \mathbb{C}^{N\times p}$ for some p.

4. Moment matching theorems. In this section, a moment matching theorem between the original transfer function (2.2) and the reduced-order transfer function (2.13) is presented. Model reduction is conducted by projecting the original system onto selected subspaces spanned by the columns of matrices $\mathbf{X} \in \mathbb{C}^{N\times N_R}$ and $\mathbf{Y} \in \mathbb{C}^{N\times N_R}$, where

$$\mathbf{l}_R = \mathbf{X}^*\mathbf{l}, \quad \mathbf{b}_R = \mathbf{Y}^*\mathbf{b}, \quad \mathbf{D}_{R,i} = \mathbf{Y}^*\mathbf{D}_i\mathbf{X} \quad \text{for } i = 1, \ldots, n \ . \tag{4.1}$$

To show moment matching properties, one classically first converts to an equivalent first order form [10, 3, 8]. Here we show such proofs are possible, even in the nth-order case without resorting to this non-unique device. Our basic tool will be projectors as utilized in Li and Bai [8]. To arrive at our main theorem, we will first introduce 3 lemmas. The first introduces two projectors related to $\mathsf{span}(\mathbf{X})$ and $\mathsf{span}(\mathbf{Y})$.

Lemma 4.1. *A matrix* $\mathbf{P} \in \mathbb{C}^{N\times N}$ *that satisfies* $\mathbf{P}^2 = \mathbf{P}$ *is defined as a projector onto* $\mathsf{span}(\mathbf{P})$. *Given matrices* $\mathbf{X}, \mathbf{Y} \in \mathbb{C}^{N\times N_R}$ *and* $\mathbf{D}_0 \in \mathbb{C}^{N\times N}$, *we define the projectors,*

$$\mathbf{P} = \mathbf{X}\left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1}\mathbf{Y}^*\mathbf{D}_0 \ , \tag{4.2}$$

$$\mathbf{Q} = \mathbf{D}_0\mathbf{X}\left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1}\mathbf{Y}^* \ , \tag{4.3}$$

where $\left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right), \mathbf{D}_0$ *are assumed invertible. Then* $\mathbf{P}$, $\mathbf{Q}$ *are projectors onto* $\mathsf{span}(\mathbf{X})$, $\mathsf{span}(\mathbf{Y})$*:*

$$\begin{aligned} \mathbf{P}\mathbf{x} &= \mathbf{x} \quad \text{for any } \mathbf{x} \in \mathsf{span}(\mathbf{X}), \\ \mathbf{y}^*\mathbf{Q} &= \mathbf{y}^* \quad \text{for any } \mathbf{y} \in \mathsf{span}(\mathbf{Y}) \ . \end{aligned} \tag{4.4}$$

Proof. This lemma is a well known fact and is stated without proof. □

Our second lemma presents some useful relations between the projectors $\mathbf{P}$ and $\mathbf{Q}$ and elements of the full and reduced-order models. In particular we identify how certain elements of the ranges of $\mathbf{X}$ and $\mathbf{Y}$ are related to elements of the unreduced model.

Lemma 4.2. *Let matrices be defined as in (2.8, 2.10, 2.16, 2.17, 4.1, 4.2, 4.3). Then for* $i = 1, \ldots, n$

$$\begin{aligned} \mathbf{X}\mathbf{D}_{R,0}^{-1}\mathbf{b}_R &= \mathbf{P}\mathbf{D}_0^{-1}\mathbf{b} \ , \\ \mathbf{X}\mathbf{A}_{R,r}^i &= \mathbf{P}\mathbf{A}_r^i\mathbf{X} \ , \\ \mathbf{l}_R^*\mathbf{D}_{R,0}^{-1}\mathbf{Y}^* &= \mathbf{l}^*\mathbf{D}_0^{-1}\mathbf{Q} \ , \\ \mathbf{A}_{R,l}^{i*}\mathbf{Y}^* &= \mathbf{Y}^*\mathbf{A}_l^{i^*}\mathbf{Q} \ . \end{aligned} \tag{4.5}$$

Proof. By (4.1, 4.2), we have

$$\begin{aligned} \mathbf{X}\mathbf{D}_{R,0}^{-1}\mathbf{b}_R &= \mathbf{X}\left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1}\mathbf{Y}^*\left(\mathbf{D}_0\mathbf{D}_0^{-1}\right)\mathbf{b} = \mathbf{P}\mathbf{D}_0^{-1}\mathbf{b} \ , \\ \mathbf{X}\mathbf{A}_{R,r}^i &= -\mathbf{X}\mathbf{D}_{R,0}^{-1}\mathbf{D}_{R,i} = -\mathbf{X}\left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1}\mathbf{Y}^*\left(\mathbf{D}_0\mathbf{D}_0^{-1}\right)\mathbf{D}_i\mathbf{X} = -\mathbf{P}\mathbf{D}_0^{-1}\mathbf{D}_i\mathbf{X} \\ &= \mathbf{P}\mathbf{A}_r^i\mathbf{X} \ . \end{aligned}$$

Similarly, by (4.1, 4.3), we have

$$\begin{aligned}
\mathbf{l}_R^* \mathbf{D}_{R,0}^{-1} \mathbf{Y}^* &= \mathbf{l}^* \left(\mathbf{D}_0^{-1}\mathbf{D}_0\right) \mathbf{X} \left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1} \mathbf{Y}^* = \mathbf{l}^* \mathbf{D}_0^{-1} \mathbf{Q} \ , \\
\mathbf{A}_{R,l}^{i*} \mathbf{Y}^* &= -\mathbf{D}_{R,i} \mathbf{D}_{R,0}^{-1} \mathbf{Y}^* = -\mathbf{Y}^* \mathbf{D}_i \left(\mathbf{D}_0^{-1}\mathbf{D}_0\right) \mathbf{X} \left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1} \mathbf{Y}^* = -\mathbf{Y}^*\mathbf{D}_i \mathbf{D}_0^{-1} \mathbf{Q} \\
&= \mathbf{Y}^* \mathbf{A}_l^{i^*} \mathbf{Q} \ .
\end{aligned}$$

∎

Our third lemma shows how elements of the moment expressions for the full system are related to elements of the reduced system via the spans of $\mathbf{X}$ and $\mathbf{Y}$.

LEMMA 4.3. *Let matrices be defined as in (2.8, 2.10, 2.16, 2.17, 4.1) with their associated sequences from Lemma 2.1. Let integers* $k, r \geq 0$. *If,*

$$\mathcal{K}_k^n \left(\{\mathbf{A}_r^i\}_{i=1}^n ; \mathbf{D}_0^{-1}\mathbf{b}\right) \subset \mathsf{span}\left(\mathbf{X}\right) \ , \tag{4.6}$$

$$\mathcal{K}_r^n \left(\{\mathbf{A}_l^i\}_{i=1}^n ; \mathbf{D}_0^{-*}\mathbf{l}\right) \subset \mathsf{span}\left(\mathbf{Y}\right) \ , \tag{4.7}$$

then

$$\mathbf{X}\mathbf{E}_{R,r}^i \mathbf{D}_{R,0}^{-1} \mathbf{b}_R = \mathbf{E}_r^i \mathbf{D}_0^{-1} \mathbf{b} \qquad (0 \leq i \leq k-1) \ , \tag{4.8}$$

$$\mathbf{l}_R^* \mathbf{D}_{R,0}^{-1} \mathbf{E}_{R,l}^{j*} \mathbf{Y}^* = \mathbf{l}^* \mathbf{D}_0^{-1} \mathbf{E}_l^{j^*} \qquad (0 \leq j \leq r-1) \ . \tag{4.9}$$

These two relations imply,

$$\mathbf{l}_R^* \mathbf{E}_{R,r}^i \mathbf{A}_{R,r}^p \mathbf{E}_{R,r}^j \mathbf{D}_{R,0}^{-1} \mathbf{b}_R = \mathbf{l}^* \mathbf{E}_r^i \mathbf{A}_r^p \mathbf{E}_r^j \mathbf{D}_0^{-1} \mathbf{b} \ , \tag{4.10}$$

for all $0 \leq i \leq k-1$, $0 \leq j \leq r-1$, *and* $1 \leq p \leq n$.

Proof. Let projectors $\mathbf{P}, \mathbf{Q}$ be defined as in (4.2,4.3). We first prove (4.8) by induction. For $i = 0$, by multiple application of Lemma 4.1, we have,

$$\begin{aligned}
\mathbf{X}\mathbf{E}_{R,r}^0 \mathbf{D}_{R,0}^{-1} \mathbf{b}_R &= \mathbf{X}\mathbf{I} \left(\mathbf{Y}^*\mathbf{D}_0\mathbf{X}\right)^{-1} \mathbf{Y}^* \left(\mathbf{D}_0\mathbf{D}_0^{-1}\right) \mathbf{b} = \mathbf{P}\mathbf{D}_0^{-1}\mathbf{b} = \mathbf{D}_0^{-1}\mathbf{b} \\
&= \mathbf{E}_r^0 \mathbf{D}_0^{-1} \mathbf{b} \ .
\end{aligned}$$

Assume the relation holds for all integers smaller than i. Then,

$$\begin{aligned}
\mathbf{X}\mathbf{E}_{R,r}^i \mathbf{D}_{R,0}^{-1} \mathbf{b}_R &= \mathbf{X} \left[\sum_{j=1}^{min(i,n)} \mathbf{A}_{R,r}^j \mathbf{E}_{R,r}^{i-j} \right] \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \sum_{j=1}^{min(i,n)} \left[\mathbf{X}\mathbf{A}_{R,r}^j\right] \mathbf{E}_{R,r}^{i-j} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \sum_{j=1}^{min(i,n)} \mathbf{P}\mathbf{A}_r^j \left[\mathbf{X}\mathbf{E}_{R,r}^{i-j} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R\right] \\
&= \sum_{j=1}^{min(i,n)} \mathbf{P}\mathbf{A}_r^j \mathbf{E}_r^{i-j} \mathbf{D}_0^{-1} \mathbf{b} \\
&= \mathbf{P} \left[\sum_{j=1}^{min(i,n)} \mathbf{A}_r^j \mathbf{E}_r^{i-j} \right] \mathbf{D}_0^{-1} \mathbf{b} \\
&= \mathbf{P}\mathbf{E}_r^i \mathbf{D}_0^{-1} \mathbf{b} \\
&= \mathbf{E}_r^i \mathbf{D}_0^{-1} \mathbf{b} \ .
\end{aligned}$$

By taking the conjugate transpose of (4.9), one obtains

$$\mathbf{Y}\mathbf{E}^i_{R,l}\mathbf{D}^{-*}_{R,0}\mathbf{l}_R = \mathbf{E}^i_l\mathbf{D}^{-*}_0\mathbf{l}\ . \tag{4.11}$$

Relation (4.9) is proved by the same procedure as (4.8) under the substitutions:

$$\begin{array}{cc} \mathbf{X} \to \mathbf{Y} & \mathbf{P} \to \mathbf{Q}^* \\ \mathbf{E}^i_{R,r} \to \mathbf{E}^i_{R,l} & \mathbf{E}^i_r \to \mathbf{E}^i_l \\ \mathbf{D}_{R,0} \to \mathbf{D}^*_{R,0} & \mathbf{D}_0 \to \mathbf{D}^*_0 \\ \mathbf{b}_R \to \mathbf{l}_R & \mathbf{b} \to \mathbf{l}\ . \end{array}$$

Since the vectors $\mathbf{b}, \mathbf{l}$ are arbitrary in the expressions for the moments in (2.11,2.15), the equalities imply that

$$\mathbf{E}^i_r\mathbf{D}^{-1}_0 = \mathbf{D}^{-1}_0\mathbf{E}^{i*}_l\ , \tag{4.12}$$

$$\mathbf{E}^i_{R,r}\mathbf{D}^{-1}_{R,0} = \mathbf{D}^{-1}_{R,0}\mathbf{E}^{i*}_{R,l}\ . \tag{4.13}$$

Relation (4.10) is obtained from these relations with the help of (4.8,4.9) as

$$\begin{aligned} \mathbf{l}^*_R\mathbf{E}^i_{R,r}\mathbf{A}^p_{R,r}\mathbf{E}^j_{R,r}\mathbf{D}^{-1}_{R,0}\mathbf{b}_R &= \mathbf{l}^*_R\mathbf{E}^i_{R,r}\left(-\mathbf{D}^{-1}_{R,0}\mathbf{D}_{R,p}\right)\mathbf{E}^j_{R,r}\mathbf{D}^{-1}_{R,0}\mathbf{b}_R \\ &= -\mathbf{l}^*_R\left(\mathbf{E}^i_{R,r}\mathbf{D}^{-1}_{R,0}\right)\left(\mathbf{Y}^*\mathbf{D}_p\mathbf{X}\right)\mathbf{E}^j_{R,r}\mathbf{D}^{-1}_{R,0}\mathbf{b}_R \\ &= -\left[\mathbf{l}^*_R\left(\mathbf{D}^{-1}_{R,0}\mathbf{E}^{i*}_{R,l}\right)\mathbf{Y}^*\right]\mathbf{D}_p\left(\mathbf{X}\mathbf{E}^j_{R,r}\mathbf{D}^{-1}_{R,0}\mathbf{b}_R\right) \\ &= -\left[\mathbf{l}^*\mathbf{D}^{-1}_0\mathbf{E}^{i*}_l\right]\mathbf{D}_p\left(\mathbf{E}^j_r\mathbf{D}^{-1}_0\mathbf{b}\right) \\ &= -\mathbf{l}^*\left(\mathbf{D}^{-1}_0\mathbf{E}^{i*}_l\right)\mathbf{D}_p\left(\mathbf{E}^j_r\mathbf{D}^{-1}_0\mathbf{b}\right) \\ &= \mathbf{l}^*\mathbf{E}^i_r\left(-\mathbf{D}^{-1}_0\mathbf{D}_p\right)\mathbf{E}^j_r\mathbf{D}^{-1}_0\mathbf{b} \\ &= \mathbf{l}^*\mathbf{E}^i_r\mathbf{A}^p_r\mathbf{E}^j_r\mathbf{D}^{-1}_0\mathbf{b}\ . \end{aligned}$$

□

We now come to our main result which proves to what extent one can match moments in reduced-order models of the nth-order systems.

Theorem 4.4. *Let matrices be defined as in (2.8, 2.10, 4.1). Let integers $k, r \geq 0$. If,*

$$\mathcal{K}^n_k\left(\{\mathbf{A}^i_r\}^n_{i=1};\mathbf{D}^{-1}_0\mathbf{b}\right) \subset \mathsf{span}\left(\mathbf{X}\right)\ , \tag{4.14}$$

$$\mathcal{K}^n_r\left(\{\mathbf{A}^i_l\}^n_{i=1};\mathbf{D}^{-*}_0\mathbf{l}\right) \subset \mathsf{span}\left(\mathbf{Y}\right)\ , \tag{4.15}$$

then

$$M_i = M_{R,i} \qquad (0 \leq i \leq k+r-1)\ . \tag{4.16}$$

This implies,

$$H(s) = H_R(s) + O\left(s^{k+r}\right)\ . \tag{4.17}$$

Proof. For $0 \le i \le k-1$ and $0 \le j \le r-1$, using Lemma 4.3, Lemma 2.1, Lemma A.2 in the Appendix we have,

$$\begin{aligned}
M_{R,i+j+1} &= \mathbf{l}_R^* \mathbf{E}_{R,r}^{i+j+1} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \mathbf{l}_R^* \left\{ \mathbf{E}_{R,r}^{i+1} \mathbf{E}_{R,r}^{j} + \sum_{l=1}^{n-1} \mathbf{E}_{R,r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{R,r}^{j-l} \right\} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \mathbf{l}_R^* \left\{ \left(\sum_{p=1}^{min(i+1,n)} \mathbf{E}_{R,r}^{i+1-p} \mathbf{A}_{R,r}^{p} \right) \mathbf{E}_{R,r}^{j} + \sum_{l=1}^{n-1} \mathbf{E}_{R,r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{R,r}^{j-l} \right\} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \sum_{p=1}^{min(i+1,n)} \mathbf{l}_R^* \mathbf{E}_{R,r}^{i+1-p} \mathbf{A}_{R,r}^{p} \mathbf{E}_{R,r}^{j} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R + \sum_{l=1}^{n-1} \mathbf{l}_R^* \mathbf{E}_{R,r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{R,r}^{j-l} \mathbf{D}_{R,0}^{-1} \mathbf{b}_R \\
&= \sum_{p=1}^{min(i+1,n)} \mathbf{l}^* \mathbf{E}_{r}^{i+1-p} \mathbf{A}_{r}^{p} \mathbf{E}_{r}^{j} \mathbf{D}_{0}^{-1} \mathbf{b} + \sum_{l=1}^{n-1} \mathbf{l}^* \mathbf{E}_{r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{r}^{j-l} \mathbf{D}_{0}^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left\{ \left(\sum_{p=1}^{min(i+1,n)} \mathbf{E}_{r}^{i+1-p} \mathbf{A}_{r}^{p} \right) \mathbf{E}_{r}^{j} + \sum_{l=1}^{n-1} \mathbf{E}_{r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{r}^{j-l} \right\} \mathbf{D}_{0}^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left\{ \mathbf{E}_{r}^{i+1} \mathbf{E}_{r}^{j} + \sum_{l=1}^{n-1} \mathbf{E}_{r}^{i+1-l} \mathbf{A}^{l+1} \mathbf{E}_{r}^{j-l} \right\} \mathbf{D}_{0}^{-1} \mathbf{b} \\
&= \mathbf{l}^* \mathbf{E}_{r}^{i+j+1} \mathbf{D}_{0}^{-1} \mathbf{b} = M_{i+j+1} \ .
\end{aligned}$$

∎

REMARK 4.1. Slone [11] in the WCAWE selects,

$$\mathcal{K}_k^n \left(\{\mathbf{A}_r^i\}_{i=1}^n ; \mathbf{D}_0^{-1} \mathbf{b} \right) = \mathsf{span}\,(\mathbf{X}) \ ,$$

and $\mathbf{X} = \mathbf{Y}$ leading to only k matched moments.

REMARK 4.2. It is often the case that one wishes to match moments not about the origin but rather near $s = s_0 \neq 0$. In this case, the nth-order transfer function (2.2) can be rewritten incorporating this shift as,

$$\begin{aligned}
H(s) &= \mathbf{l}^* \left(\sum_{i=0}^{n} s^i \mathbf{D}_i \right)^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left[\sum_{i=0}^{n} \{ s_0 + (s - s_0) \}^i \mathbf{D}_i \right]^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left[\sum_{i=0}^{n} \sum_{p=0}^{i} \begin{pmatrix} i \\ p \end{pmatrix} s_0^{i-p} (s - s_0)^p \mathbf{D}_i \right]^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left[\sum_{p=0}^{n} \left\{ \sum_{i=p}^{n} \begin{pmatrix} i \\ p \end{pmatrix} s_0^{i-p} \mathbf{D}_i \right\} (s - s_0)^p \right]^{-1} \mathbf{b} \\
&= \mathbf{l}^* \left[\sum_{p=0}^{n} \widehat{\mathbf{D}}_p (s - s_0)^p \right]^{-1} \mathbf{b} \ , \qquad (4.18)
\end{aligned}$$

where we have defined,

$$\widehat{\mathbf{D}}_p := \sum_{i=p}^{n} \begin{pmatrix} i \\ p \end{pmatrix} s_0^{i-p}\mathbf{D}_i \text{ , for } p = 1, \ldots, n \quad , \tag{4.19}$$

$$\begin{pmatrix} i \\ p \end{pmatrix} := \frac{i!}{p!(i-p)!} \ . \tag{4.20}$$

Application of Theorem 4.4 to the case incorporating a shift s_0 results in the following corollary.

COROLLARY 4.5. *Let integers $k, r \geq 0$. Let matrices be defined as in (4.1, 4.19). Additionally define,*

$$\widehat{\mathbf{D}}_{R,i} = \mathbf{Y}^* \widehat{\mathbf{D}}_i \mathbf{X} \ , \tag{4.21}$$

If,

$$\mathcal{K}_k^n \left(\left\{ \widehat{\mathbf{D}}_0^{-1} \widehat{\mathbf{D}}_i \right\}_{i=1}^{n} ; \widehat{\mathbf{D}}_0^{-1}\mathbf{b} \right) \subset \mathsf{span}\left(\mathbf{X}\right) \tag{4.22}$$

$$\mathcal{K}_r^n \left(\left\{ \widehat{\mathbf{D}}_0^{-*} \widehat{\mathbf{D}}_i^* \right\}_{i=1}^{n} ; \widehat{\mathbf{D}}_0^{-*}\mathbf{l} \right) \subset \mathsf{span}\left(\mathbf{Y}\right) \tag{4.23}$$

then

$$M_i(s_0) = M_{R,i}(s_0) \qquad (0 \leq i \leq k + r - 1) \ , \tag{4.24}$$

where,

$$M_i(s_0) = \mathbf{l}^* \widehat{\mathbf{E}}_r^i \widehat{\mathbf{D}}_0^{-1} \mathbf{b} \qquad = \mathbf{l}^* \widehat{\mathbf{D}}_0^{-1} \widehat{\mathbf{E}}_l^{i*} \mathbf{b} \tag{4.25}$$

$$M_{Ri}(s_0) = \mathbf{l}_R^* \widehat{\mathbf{E}}_{R,r}^i \widehat{\mathbf{D}}_{R,0}^{-1} \mathbf{b}_R = \mathbf{l}_R^* \widehat{\mathbf{D}}_{R,0}^{-1} \widehat{\mathbf{E}}_{R,l}^{i*} \mathbf{b}_R \ . \tag{4.26}$$

This implies,

$$H(s) = H_R(s) + O\left((s - s_0)^{k+r} \right) \ . \tag{4.27}$$

REMARK 4.3. The theorem and corollary presented also apply to the case of a MIMO system by replacing the input distribution vector $\mathbf{b}$ with an input distribution matrix $\mathbf{B} \in \mathbb{C}^{N \times p}$, and by replacing the output distribution vector $\mathbf{l}$ with an output distribution matrix $\mathbf{L} \in \mathbb{C}^{N \times p}$, for some p.

REMARK 4.4. Consider the transfer function of a SISO first-order system,

$$H(s) = \mathbf{l}^* \left(\mathbf{G} + s\mathbf{C} \right)^{-1} \mathbf{b} \ ,$$

where $\mathbf{l}, \mathbf{b} \in \mathbb{C}^{N \times N}$ and $\mathbf{G}, \mathbf{C} \in \mathbb{C}^{N \times N}$. One can identify,

$$\mathbf{D}_0 = \mathbf{G}, \quad \mathbf{A}_r^1 = -\mathbf{G}^{-1}\mathbf{C}, \quad \mathbf{A}_l^1 = -\mathbf{G}^{-*}\mathbf{C}^*.$$

The application of Theorem 4.4 with $n = 1$ yields the exact same results as Theorem 3.3 of [8] and other moment matching theorems presented for first-order systems [13, 7, 10].

5. Connections between Krylov subspaces. The standard method of treating a higher-order systems is to transform it to an equivalent first-order system. Here we elaborate on the connections between the nth-order Krylov subspace and standard Krylov subspaces obtained from two types of equivalent first-order forms. For comparison with general equivalent first-order forms, one must look at vector spaces of linearizations and the standard Krylov subspaces they generate [9].

LEMMA 5.1. *Given the transfer function for an nth-order system,*

$$H(s) = \mathbf{l}^* \left(\sum_{i=0}^{n} (s - s_0)^i \widehat{\mathbf{D}}^i \right)^{-1} \mathbf{b} \ ,$$

where $\widehat{\mathbf{D}}_i$ is defined in (4.19), one can rewrite this as an equivalent first order system,

$$H(s) = \mathbf{l}_f^* \left((s - s_0)\mathbf{C} + \mathbf{G} \right)^{-1} \mathbf{b}_f, \tag{5.1}$$

where $\mathbf{l}_f, \mathbf{b}_f \in \mathbb{C}^{Nn}$ and $\mathbf{C}, \mathbf{G} \in \mathbb{C}^{Nn \times Nn}$ are defined as,

$$\mathbf{l}_f := \begin{bmatrix} \mathbf{l} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}, \qquad \mathbf{b}_f := \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{G} := \begin{bmatrix} \widehat{\mathbf{D}}_0 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{W}_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{W}_{n-1} \end{bmatrix}, \tag{5.2}$$

$$\mathbf{C} := \begin{bmatrix} \widehat{\mathbf{D}}_1 & \widehat{\mathbf{D}}_2 & \widehat{\mathbf{D}}_3 & \cdots & \widehat{\mathbf{D}}_n \\ -\mathbf{W}_1 & \mathbf{0} & \mathbf{0} & \ddots & \vdots \\ \mathbf{0} & -\mathbf{W}_2 & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & -\mathbf{W}_{n-1} & \mathbf{0} \end{bmatrix} . \tag{5.3}$$

Here $\mathbf{W}_i \in \mathbb{C}^{N \times N}$, $i = 1, , \ldots, n-1$ are non-singular matrices. Denote the kth standard Krylov subspaces defined by the equivalent first-order system as,

$$\mathcal{K}_k(-\mathbf{G}^{-1}\mathbf{C}; \mathbf{G}^{-1}\mathbf{b}_f) = \mathsf{span}(\mathbf{X}) = \mathsf{span}\left(\begin{bmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_n \end{bmatrix} \right), \tag{5.4}$$

$$\mathcal{K}_k(-\mathbf{G}^{-*}\mathbf{C}^*; \mathbf{G}^{-*}\mathbf{l}_f) = \mathsf{span}(\mathbf{Y}) = \mathsf{span}\left(\begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_n \end{bmatrix} \right), \tag{5.5}$$

where $\mathbf{X}, \mathbf{Y} \in \mathbb{C}^{Nn \times k}$ and $\mathbf{X}_i, \mathbf{Y}_i \in \mathbb{C}^{N \times k}$, $(i = 1, \ldots, n)$. The columns of the matrices $\mathbf{X}$ and $\mathbf{Y}$ correspond to the Krylov vectors. When $\mathbf{W}_i = \widehat{\mathbf{D}}_0$, $(i = 1, \ldots, n-1)$,

$$\mathsf{span}(\mathbf{X}_1) = \mathcal{K}_k^n \left(\{-\widehat{\mathbf{D}}_0^{-1} \widehat{\mathbf{D}}_i\}_{i=1}^n ; \widehat{\mathbf{D}}_0^{-1} \mathbf{b} \right), \tag{5.6}$$

$$\mathsf{span}(\mathbf{Y}_1) = \mathcal{K}_k^n \left(\{-\widehat{\mathbf{D}}_0^{-*} \widehat{\mathbf{D}}_i^*\}_{i=1}^n ; \widehat{\mathbf{D}}_0^{-*} \mathbf{l} \right), \tag{5.7}$$

and,

$$\mathsf{span}\,(\mathbf{X}_i) \subset \mathsf{span}\,(\mathbf{X}_1) \quad \text{for } i = 2, \ldots, n \quad . \tag{5.8}$$

The columns of the matrices $\mathbf{X}_1$ *and* $\mathbf{Y}_1$ *correspond to the sequence of vectors generated by the kth nth-order Krylov subspace.*

Proof. We have,

$$-\mathbf{G}^{-1}\mathbf{C} = \begin{bmatrix} -\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_1 & -\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_2 & -\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_3 & \cdots & -\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_n \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{I} & \mathbf{0} \end{bmatrix} , \tag{5.9}$$

$$-\mathbf{G}^{-*}\mathbf{C}^* = \begin{bmatrix} -\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_1^* & \mathbf{I} & \mathbf{0} & \cdots & \mathbf{0} \\ -\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_2^* & \mathbf{0} & \mathbf{I} & \ddots & \vdots \\ -\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_3^* & \mathbf{0} & \mathbf{0} & \ddots & \mathbf{0} \\ \vdots & \vdots & \ddots & \ddots & \mathbf{I} \\ -\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_n^* & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} \end{bmatrix} , \tag{5.10}$$

$$-\mathbf{G}^{-1}\mathbf{b}_f = \begin{bmatrix} \widehat{\mathbf{D}}_0^{-1}\mathbf{b} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} , -\mathbf{G}^{-*}\mathbf{l}_f = \begin{bmatrix} \widehat{\mathbf{D}}_0^{-*}\mathbf{l} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} . \tag{5.11}$$

By denoting $\mathbf{x}_{i,j} \in \mathbb{C}^N$ as the jth column of $\mathbf{X}_i$, from

$$\begin{bmatrix} \mathbf{x}_{1,j+1} \\ \vdots \\ \mathbf{x}_{n,j+1} \end{bmatrix} = \left(-\mathbf{G}^{-1}\mathbf{C}\right) \begin{bmatrix} \mathbf{x}_{1,j} \\ \vdots \\ \mathbf{x}_{n,j} \end{bmatrix} \quad (1 \le j \le k-1),$$

we have the recursion relation,

$$\begin{aligned} \mathbf{x}_{1,j+1} &= \textstyle\sum_{i=1}^n \left(-\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_i\right)\mathbf{x}_{i,j} & & (1 \le j \le k-1), \\ \mathbf{x}_{i,j+1} &= \mathbf{x}_{i-1,j} & (2 \le i \le n, & \quad 1 \le j \le k-1). \end{aligned} \tag{5.12}$$

Since,

$$\mathbf{x}_{i,j} = \mathbf{x}_{i-1,j-1} \qquad (2 \le i \le n, 2 \le j \le k-1),$$

the sequence $\{\mathbf{x}_{1,j}\}$ can be expressed as,

$$\begin{aligned} \mathbf{x}_{1,j} &= \sum_{i=1}^{min(j-1,n)} \left(-\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_i\right)\mathbf{x}_{i-(i-1),j-1-(i-1)} \\ &= \sum_{i=1}^{min(j-1,n)} \left(-\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_i\right)\mathbf{x}_{1,j-i} \qquad (2 \le j). \end{aligned} \tag{5.13}$$

The recursion relation for the sequence $\{\mathbf{x}_{1,j}\}_{j=1}^{k}$ (5.13) is identical to the kth nth-order Krylov subspace, $\mathcal{K}_k^n\left(\{-\widehat{\mathbf{D}}_0^{-1}\widehat{\mathbf{D}}_i\}_{i=1}^n; \widehat{\mathbf{D}}_0^{-1}\mathbf{b}\right)$. Clearly from (5.12), the sequences $\{\mathbf{x}_{i,j}\}_{j=1}^{k}$, for $i = 2, \ldots, n$ are subsequences of $\{\mathbf{x}_{1,j}\}_{j=1}^{k}$. This proves (5.6) and (5.8).

Similarly by denoting $\mathbf{y}_{i,j} \in \mathbb{C}^N$ as the jth column of $\mathbf{Y}_i$, from

$$\begin{bmatrix} \mathbf{y}_{1,j+1} \\ \vdots \\ \mathbf{y}_{n,j+1} \end{bmatrix} = \left(-\mathbf{G}^{-*}\mathbf{C}^*\right) \begin{bmatrix} \mathbf{y}_{1,j} \\ \vdots \\ \mathbf{y}_{n,j} \end{bmatrix} \quad (1 \le j \le k-1),$$

we have the recursion relation,

$$\begin{aligned} \mathbf{y}_{i,j+1} &= \left(-\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_i^*\right)\mathbf{y}_{1,j} + \mathbf{y}_{i+1,j} \quad (1 \le i \le n-1, \quad 1 \le j \le k-1), \\ \mathbf{y}_{n,j+1} &= \left(-\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_i^*\right)\mathbf{y}_{1,j} \quad (1 \le i \le n-1). \end{aligned} \tag{5.14}$$

Since,

$$\mathbf{y}_{i,j+1} - \mathbf{y}_{i+1,j} = \left(-\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_i^*\right)\mathbf{y}_{1,j} \qquad (1 \le i \le n-1,\ 1 \le j \le k-1),$$

we have,

$$\mathbf{y}_{1,j} = \sum_{i=1}^{min(j-1,n)} \left(-\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_i^*\right)\mathbf{y}_{1,j-i}. \tag{5.15}$$

The recursion relation for the sequence $\{\mathbf{y}_{1,j}\}_{j=0}^{k-1}$ (5.15) is identical to the kth nth-order Krylov subspace, $\mathcal{K}_k^n\left(\{-\widehat{\mathbf{D}}_0^{-*}\widehat{\mathbf{D}}_i^*\}_{i=1}^n; \widehat{\mathbf{D}}_0^{-*}\mathbf{l}\right)$. This proves (5.7). □

REMARK 5.1. The relationship (5.8) has already been noted in [8, 11]. For the second-order system, the relationship (5.6) combined with (5.8) has been denoted as the embedding of the second-order Krylov subspace in the standard Krylov-subspace generated from the equivalent first-order system. In Remark 6.2. of [8], it is mentioned that Theorem 5.2. of [8] is enough to extend their moment-matching theorem for first-order systems to higher-order systems. This is not fully precise since the block structure of $-\mathbf{G}^{-*}\mathbf{C}^*$ is different from that of $-\mathbf{G}^{-1}\mathbf{C}$. Relation (5.7) is needed to fully establish their claim.

REMARK 5.2. The equivalent first-order system here has been constructed by the shift-"before"-linearization procedure. In this procedure, the effect of the nonzero shift s_0 is taken into account before forming the equivalent first-order system. Lemma 5.1 states that by selecting a particular form of the first-order system and conducting a shift-"before"-linearization, the 1st block of the standard Krylov subspace generated by the equivalent first-order system spans the same subspace as the kth nth-order Krylov subspaces independent of the value of the shift s_0. This implies that the nth-order Krylov subspaces can be constructed by generating the standard Krylov subspaces of the equivalent first-order form and then extracting the necessary components.

REMARK 5.3. By observing the block structure of $-\mathbf{G}^{-1}\mathbf{C}$, one can see that this does not conform to the block structure required for application of the theorem by Freund [6]. This discrepancy arises from the difference between shift-"before"-linearization and shift-"after"-linearization. Since the matrices are different, the standard Krylov subspaces generated by the two equivalent first-order systems are different. But still one can prove that the 1st block of the standard Krylov subspaces span the same subspace, and thus correspond to the nth-order Krylov subspace. In the shift-"after"-linearization used by Freund, the matrices have the following form,

$$\mathbf{M}^i := -\widehat{\mathbf{D}}_0^{-1}\sum_{j=0}^{l-i} s_0^j \mathbf{D}_{i+j}, \quad i = 1, 2, \dots, l, \tag{5.16}$$

$$-\mathbf{G}_F^{-1}\mathbf{C}_F = \begin{bmatrix} \mathbf{M}^1 & \mathbf{M}^2 & \mathbf{M}^3 & \cdots & \mathbf{M}^n \\ s_0\mathbf{M}^1 & s_0\mathbf{M}^2 & s_0\mathbf{M}^3 & \cdots & s_0\mathbf{M}^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s_0^{n-1}\mathbf{M}^1 & s_0^{n-1}\mathbf{M}^2 & s_0^{n-1}\mathbf{M}^3 & \cdots & s_0^{n-1}\mathbf{M}^n \end{bmatrix} + \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ \mathbf{I} & 0 & \ddots & & \vdots \\ s_0\mathbf{I} & \mathbf{I} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ s_0^{n-2}\mathbf{I} & \cdots & s_0\mathbf{I} & \mathbf{I} & 0 \end{bmatrix}, \tag{5.17}$$

$$\mathbf{b}_{fF} = \begin{bmatrix} \mathbf{b} \\ s_0\mathbf{b} \\ \vdots \\ s_0^{n-1}\mathbf{b} \end{bmatrix}, \quad \mathbf{G}_F^{-1}\mathbf{b}_{fF} = \begin{bmatrix} \mathbf{I} \\ s_0\mathbf{I} \\ \vdots \\ s_0^{n-1}\mathbf{I} \end{bmatrix} \widehat{\mathbf{D}}_0^{-1}\mathbf{b} \; . \tag{5.18}$$

Let us define the matrix $\mathbf{X}^F \in \mathbb{C}^{Nn\times k}$,

$$\mathbf{X}^F = \begin{bmatrix} \mathbf{X}_1^F \\ \vdots \\ \mathbf{X}_n^F \end{bmatrix} . \tag{5.19}$$

whose columns span the standard Krylov subspace $\mathcal{K}_k(-\mathbf{G}_F^{-1}\mathbf{G}_F; \mathbf{G}_F^{-1}\mathbf{b}_{fF})$. By denoting $\mathbf{x}_{i,j}^F \in \mathbb{C}^N$ as the jth column of $\mathbf{X}_i^F$, from

$$\begin{bmatrix} \mathbf{x}_{1,j+1}^F \\ \vdots \\ \mathbf{x}_{n,j+1}^F \end{bmatrix} = \left(-\mathbf{G}_F^{-1}\mathbf{C}_F\right) \begin{bmatrix} \mathbf{x}_{1,j}^F \\ \vdots \\ \mathbf{x}_{n,j}^F \end{bmatrix} \quad (1 \le j \le k-1),$$

we have the recursion relation for,

$$\begin{aligned} \mathbf{x}_{i,j}^F &= \sum_{k=0}^{min(j-1,i-1)} \begin{pmatrix} i-1 \\ k \end{pmatrix} \mathbf{x}_{1,j-k}^F s_0^{i-1-k} \quad (1 \le i \le n, \quad 1 \le j \le k), \\ \mathbf{x}_{1,j}^F &= \sum_{i=1}^{n} \mathbf{M}^i \mathbf{x}_{i,j-1}^F \qquad (2 \le j \le k). \end{aligned} \tag{5.20}$$

This yields the same expression for the sequence $\{\mathbf{x}_{1,j}^F\}_{j=1}^k$ as (5.13). Thus we see that,

$$\mathsf{span}(\mathbf{X}_1) = \mathsf{span}(\mathbf{X}_1^F)\ , \tag{5.21}$$

$$\mathsf{span}(\mathbf{X}_i^F) \subset \mathsf{span}(\mathbf{X}_1^F), \quad i = 2, \ldots, n\ . \tag{5.22}$$

This result implies that it does not matter whether one conducts a shift- "before" -linearization or shift- "after" -linearization as long as the 1st block of the generated standard Krylov subspace is extracted. Though it is not proven here, numerically it is also observed that for equivalent first-order systems which are called companion forms, the columns of the 1st block span the nth-order Krylov subspace. One can further remark that since shift-"before"-linearization results in a sparser matrix, it is computationally more efficient.

REMARK 5.4. Due to the inclusion of the nth-order Krylov subspaces in the first block of $\mathbf{X}$ and $\mathbf{Y}$, one can always construct projection subspaces spanned by the columns of the matrices $\widetilde{\mathbf{X}}$ and $\widetilde{\mathbf{Y}}$,

$$\widetilde{\mathbf{X}} := \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{X}_1 \end{bmatrix} , \widetilde{\mathbf{Y}} := \begin{bmatrix} \mathbf{Y}_1 & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \mathbf{Y}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{Y}_n \end{bmatrix}, \tag{5.23}$$

such that,

$$\mathsf{span}(\mathbf{X}) \subset \mathsf{span}(\widetilde{\mathbf{X}}), \quad \mathsf{span}(\mathbf{Y}) \subset \mathsf{span}(\widetilde{\mathbf{Y}}). \tag{5.24}$$

Projecting the coefficient matrices $\mathbf{C}$ and $\mathbf{G}$ of the equivalent first-order system onto these subspaces, and then converting back to the original nth-order system results in coefficient matrices which coincide with those obtained from projecting the nth-order system onto the nth-order Krylov subspaces. This type of projection has been conducted for the second-order case in [8, 12, 10].

REMARK 5.5. The most general transfer function, whose output depends linearly on derivatives of the state space variable $\mathbf{x}$, can be expressed as,

$$\mathbf{H}(s) = \left(\sum_{i=0}^{n-1} s^i \mathbf{V}_i^*\right)\left(\sum_{i=0}^{n} s^i \mathbf{D}_i\right)^{-1} \mathbf{B}, \tag{5.25}$$

where $\mathbf{B} \in \mathbb{C}^{N\times p}$ for some p and $\{\mathbf{V}_i \in \mathbb{C}^{N\times q}\}_{i=0}^{n-1}$ for some q. In this case one must construct $\mathbf{X}$ and $\mathbf{Y}$ such that,

$$\mathcal{K}_k^n\left(\{\mathbf{A}_r^i\}_{i=1}^n; \mathbf{D}_0^{-1}\mathbf{B}\right) \subset \mathsf{span}\left(\mathbf{X}\right)\ , \tag{5.26}$$

$$\mathcal{K}_r^n\left(\{\mathbf{A}_l^i\}_{i=1}^n; \mathbf{D}_0^{-*}[\mathbf{V}_1, \cdots, \mathbf{V}_{n-1}]\right) \subset \mathsf{span}\left(\mathbf{Y}\right)\ , \tag{5.27}$$

for $k + r$ moment matching.

6. Concluding Remarks. We have presented moment matching theorems for nth-order linear dynamical systems in the context of nth-order Krylov subspaces. The definition that is provided for nth-order Krylov subspaces is a generalization of standard Krylov subspaces to higher-order systems. The main theorem states that if the right and left projection subspaces in the Krylov subspace based model reduction include the nth-order Krylov subspaces, then one can obtain the desired moment matching properties. The theorem is stated for the nth-order system without the need for a transformation to an equivalent first-order system. This eliminates complications of linearization involving selection of matrices and auxiliary variables. An additional advantage is preservation of the nth-order system in the model reduction, as well as preservation of the structure of the coefficient matrices. We have also shown the connections between the nth-order Krylov subspace and standard Krylov subspaces generated from selected equivalent first-order systems. The nth-order Krylov subspace is contained as the 1st block in the standard Krylov subspaces generated. This justifies the use of standard Krylov subspaces as a tool for generating the nth-order Krylov subspace. It has also been shown that for a particular equivalent first-order system, the differences of shift-"before"-linearization and shift-"after"-lineariztion are functionally irrelevant, in that the columns of the 1st block still span the nth-order Krylov subspace generated incorporating the shift.

Appendix.

LEMMA A.1. *Define the matrix valued functions* $f, g : \mathbb{C} \to \mathbb{C}^{N\times N}$,

$$\begin{aligned} g(s) &= \mathbf{I} - \sum_{i=1}^{n} s^i \mathbf{A}^i, \\ f(s) &= g(s)^{-1}, \end{aligned} \tag{A.1}$$

where $\mathbf{A}^i \in \mathbb{C}^{N\times N}$, $1 \le i \le n$, *are given matrices. Then the coefficients* $\mathbf{E}^i \in \mathbb{C}^{N\times N}$ *of the Taylor series expansion of* $f(s)$ *at* $s = 0$,

$$f(s) = \sum_{i=0}^{\infty} \mathbf{E}^i s^i \ , \tag{A.2}$$

are given by the recursion,

$$\mathbf{E}^0 = \mathbf{I}, \tag{A.3}$$

$$\mathbf{E}^k = \sum_{i=1}^{min(k,n)} \mathbf{A}^i \quad \mathbf{E}^{k-i} \quad (1 \le k) \tag{A.4}$$

$$= \sum_{i=1}^{min(k,n)} \mathbf{E}^{k-i} \quad \mathbf{A}^i \quad (1 \le k) \ . \tag{A.5}$$

Proof. Since $g(s)$ is of nth-order, all derivatives of order $n+1$ and higher are zero. Evaluating these at $s = 0$, we have,

$$g(0) = \mathbf{I}, \qquad g^{(k)}(0) = -k!\mathbf{A}^k \quad (1 \le k \le n).$$

By taking the derivatives of the equation $f(s)g(s) = g(s)f(s) = \mathbf{I}$ with respect to s and evaluating them at $s = 0$, we obtain the recursion,

$$\begin{aligned} f(0) &= \mathbf{I}, \\ f^{(k)}(0) &= \sum_{i=1}^{\min(k,n)} \frac{k!}{(k-i)!} \ f^{k-i}(0) \ \ \mathbf{A}^i \quad (1 \le k) \\ &= \sum_{i=1}^{\min(k,n)} \frac{k!}{(k-i)!} \ \mathbf{A}^i \ \ f^{k-i}(0) \quad (1 \le k) \ . \end{aligned}$$

Since the coefficients of the Taylor series are defined as,

$$\mathbf{E}^k = \frac{1}{k!} f^{(k)}(0) \ ,$$

the recursion relation holds. ∎

LEMMA A.2. *Let* $\{\mathbf{E}^i\}_{i=0}^{\infty}$ *be the sequence of matrices defined in Lemma A.1. Let us additionally define,*

$$\mathbf{E}^{-k} = \mathbf{0} \qquad (1 \leq k < n) \ . \tag{A.6}$$

Then,

$$\mathbf{E}^{i+j} = \mathbf{E}^i \mathbf{E}^j + \sum_{l=1}^{n-1} \mathbf{E}^{i-l} \mathbf{A}^{l+1} \mathbf{E}^{j-l} \ , \tag{A.7}$$

for all $i, j \geq 0$.

Proof. We prove this by induction. For $i, j = 0$,

$$\mathbf{E}^0 = \mathbf{E}^0 \mathbf{E}^0 = \mathbf{I} \ .$$

Assume the relation holds for $0 \leq i \leq k$ and $0 \leq j \leq r$. From Equation (A.4),

$$\begin{aligned}
\mathbf{E}^{(k+1)+r} &= \sum_{i=1}^{\min(k+1+r,n)} \mathbf{A}^i \ \mathbf{E}^{(k+1+r)-i} \\
&= \sum_{i=1}^{\min(k+1+r,n)} \mathbf{A}^i \ \left[\mathbf{E}^{k+1-i} \mathbf{E}^r + \sum_{l=1}^{n-1} \mathbf{E}^{(k+1-i)-l} \mathbf{A}^{l+1} \mathbf{E}^{r-l} \right] \\
&= \left[\sum_{i=1}^{\min(k+1+r,n)} \mathbf{A}^i \ \mathbf{E}^{k+1-i} \right] \mathbf{E}^r \\
&\quad + \left[\sum_{i=1}^{\min(k+1+r,n)} \mathbf{A}^i \ \sum_{l=1}^{n-1} \mathbf{E}^{(k+1-i)-l} \mathbf{A}^{l+1} \mathbf{E}^{r-l} \right] \\
&= \mathbf{E}^{k+1} \mathbf{E}^r + \sum_{l=1}^{n-1} \left[\sum_{i=1}^{\min(k+1+r,n)} \mathbf{A}^i \ \mathbf{E}^{(k+1-l)-i} \right] \mathbf{A}^{l+1} \ \mathbf{E}^{r-l} \\
&= \mathbf{E}^{k+1} \mathbf{E}^r + \sum_{l=1}^{n-1} \mathbf{E}^{k+1-l} \mathbf{A}^{l+1} \ \mathbf{E}^{r-l} \ .
\end{aligned}$$

and we see that the relation holds for $0 \leq i \leq k+1$ and $0 \leq j \leq r$. Similarly, from Equation (A.5),

$$\mathbf{E}^{k+(r+1)} = \sum_{i=1}^{\min(k+r+1,n)} \mathbf{E}^{(k+r+1)-i} \ \mathbf{A}^i$$

$$
\begin{aligned}
&= \sum_{i=1}^{\min(k+r+1,n)} \left[\mathbf{E}^k \mathbf{E}^{r+1-i} + \sum_{l=1}^{n-1} \mathbf{E}^{k-l} \mathbf{A}^{l+1} \mathbf{E}^{(r+1-i)-l} \right] \mathbf{A}^i \\
&= \mathbf{E}^k \left[\sum_{i=1}^{\min(k+r+1,n)} \mathbf{E}^{r+1-i} \mathbf{A}^i \right] \\
&\quad + \left[\sum_{i=1}^{\min(k+r+1,n)} \sum_{l=1}^{n-1} \mathbf{E}^{k-l} \mathbf{A}^{l+1} \mathbf{E}^{(r+1-i)-l} \mathbf{A}^i \right] \\
&= \mathbf{E}^k \mathbf{E}^{r+1} + \sum_{l=1}^{n-1} \mathbf{E}^{k-l} \mathbf{A}^{l+1} \left[\sum_{i=1}^{\min(k+1+r,n)} \mathbf{E}^{r+1-l-i} \mathbf{A}^i \right] \\
&= \mathbf{E}^k \mathbf{E}^{r+1} + \sum_{l=1}^{n-1} \mathbf{E}^{k-l} \mathbf{A}^{l+1} \mathbf{E}^{r+1-l} .
\end{aligned}
$$

and we see that the relation holds for $0 \le i \le k$ and $0 \le j \le r+1$. Combining these two, the relation holds by induction. ∎

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