PADÉ APPROXIMATION OF LARGE-SCALE DYNAMIC SYSTEMS WITH LANCZOS METHODS *

K. Gallivan, E. Grimme and P. Van Dooren

Coordinated Science Laboratory University of Illinois at Urbana-Champaign 1308 West Main Street Urbana, IL 61801

Abstract

The utility of Lanczos methods for the approximation of large-scale dynamical systems is considered. In particular, it is shown that the Lanczos method is a technique for yielding Padé approximants which has several advantages over more traditional explicit moment matching approaches. An extension of the Lanczos algorithm is developed for computing multi-point Padé approximations of descriptor systems.*

Keywords: Dynamic system, Padé approximation, Lanczos algorithm, model reduction.

1. Introduction

This paper explores the use of Lanczos techniques for the reduced-order modeling and simulation of large-scale, SISO dynamical systems. One can define such a system through the set of state space equations

$$\begin{aligned} \mathbf{E}\dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{b}u(t) \\ y(t) &= \mathbf{c}\mathbf{x}(t) + du(t). \end{aligned}$$
(1)

The scalar functions u(t) and y(t) are the system's input and output while $\mathbf{x}(t)$ is the state vector of dimension n. For simplicity, the direct-coupling term, d, will be assumed to be zero. The system matrix, $\mathbf{A} \in \mathbf{R}^{n \times n}$, and descriptor matrix, $\mathbf{E} \in \mathbf{R}^{n \times n}$, are assumed to be sparse or structured (e.g., Toeplitz). We stress that this last assumption is met by large-scale problems arising from most applications.

For the case where **E** is an identity matrix, the zerostate $(\mathbf{x}(0) = 0)$ solution to the first expression in (1) is $\mathbf{x}(t) = \int_0^t e^{\mathbf{A}(t-\tau)} \mathbf{b} u(\tau) d\tau$. Thus determining a good $k \ll n$ order approximation,

$$\begin{cases} \dot{\hat{\mathbf{x}}}(t) &= \hat{\mathbf{A}}\hat{\mathbf{x}}(t) + \hat{\mathbf{b}}u(t) \\ \hat{y}(t) &= \hat{\mathbf{c}}\hat{\mathbf{x}}(t), \end{cases}$$
(2)

is intimately connected with finding a pair $\{\hat{A}, \hat{b}\}$ which yields a good approximation to the matrix exponential,

 $e^{\mathbf{A}t}\mathbf{b}$. A method based on orthogonal Krylov projectors (the Arnoldi algorithm) is utilized in [9, 22] for approximating $e^{\mathbf{A}t}\mathbf{b}$. But in fact, these concepts can be taken one step further by noting that one is really only interested in that information in $e^{\mathbf{A}t}\mathbf{b}$ which lies in the direction of **c** (one ultimately desires $||y - \hat{y}||$ small for some desired range of inputs u). Numerous papers [2, 15, 23, 24] are beginning to explore this last fact in the context of control. In particular, these papers begin to investigate the use of an oblique Krylov projector (i.e., the Lanczos algorithm) for generating the reduced-order system $\{\hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$.

Intertwined with the Krylov projections performed in all of these papers is the Padé approximation of the transfer function, $h(s) = \mathbf{c}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{b}$. It is known [11, 25] that Krylov projections yield Padé approximations without explicitly using moments. The Lanczos method requires approximately the same amount of effort as existing, explicit moment matching techniques [7]. More importantly, the Lanczos method provides the flexibility needed to efficiently handle many of the shortcomings of Padé approximants, e.g.,

- 1. a loss of accuracy as k increases due to the power method aspects of explicit moment matching,
- singularities in the Padé table (ill-conditioned leading submatrices in the system's Hankel matrix) [18],
- 3. poor approximation of the frequency response of (1) away from the Padé expansion frequency, s_0 ,
- 4. unstable approximations of stable systems [3].

In §2, existing Lanczos techniques for the case $\mathbf{E} = \mathbf{I}$ are briefly reviewed. It is demonstrated that the Lanczos method provides the means to treat the first two shortcomings. In §3, an extension of the Lanczos method is developed for a general descriptor matrix, \mathbf{E} . Additionally, this new variant implicitly matches moments about multiple expansion frequencies (*multi-point* Padé approximation). Practical experience [19, 26] suggests that moment matching about multiple frequencies provides sufficient information to treat the third and fourth of the listed shortcomings.

These results are of interest to any application currently utilizing Padé approximants of dynamical systems. For example, asymptotic waveform evaluation (AWE) is a recently developed technique for acquiring low-order Padé approximations for large, linearized circuits [19]. However, existing

^{*}This work has been supported in part by the National Science Foundation under grants CCR-9120105 and CCR-9209349. The work of the second author was also supported in part by a DOE Computational Science Graduate Fellowship.

^{*}Also available in Procs. IEEE 33rd Conf. on Decision and Control, pp. 443–448.

AWE papers do not link Krylov projectors and Padé approximation together.

2. Padé approximation with Lanczos methods

In conventional Padé techniques [5], an approximation for the dynamical system (1) is typically obtained through a two-step process. First, moments which correspond to frequency domain expansions of the circuit's impulse response are explicitly computed. Most commonly, the expansion is performed either about $s_0 = 0$ to yield the low-frequency moments, $m_j = \mathbf{c}\mathbf{A}^{-j-1}\mathbf{b}, \ j \ge 0$, or about $s_0 = \infty$ to yield the high-frequency moments (Markov parameters), $m_j = \mathbf{c}\mathbf{A}^{-j-1}\mathbf{b}, \ j < 0$. In the second step, the impulse response

$$\hat{h}(s) = \frac{n_{k-1}s^{k-1} + \ldots + n_1s + n_0}{s_k + d_{k-1}s^{k-1} + \ldots + d_1s + d_0}$$
(3)

of the approximate realization is chosen so that 2k moments of the original system are matched. In particular, a linear system of equations of the form $\mathbf{Md} = \mathbf{m}$ is solved where \mathbf{M} is a Hankel matrix whose elements are the moments, m_j . Note that given (3), is is not difficult to obtain some state space realization $\{\hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$. The order-k system which matches 2k moments of the original system is said to be a partial realization. The impulse response corresponding to the partial realization is a Padé approximant.

As an alternative to explicit moment matching, consider using the oblique Krylov projector $\pi_k = \pi_k^2 = \mathbf{V}_k \mathbf{W}_k^T$ to produce a k^{th} order model,

$$\begin{cases} \dot{\hat{\mathbf{x}}} = (\mathbf{W}_k^T \mathbf{A} \mathbf{V}_k) \hat{\mathbf{x}} + (\mathbf{W}_k^T \mathbf{b}) u = \hat{\mathbf{A}} \hat{\mathbf{x}} + \hat{\mathbf{b}} u \\ \hat{\mathbf{y}} = (\mathbf{c} \mathbf{V}_k) \hat{\mathbf{x}} = \hat{\mathbf{c}} \hat{\mathbf{x}}, \end{cases}$$
(4)

for the original system (1), see [24]. The matrices \mathbf{V}_k and \mathbf{W}_k are related to Krylov spaces, \mathcal{K}_k , in that

$$COLSP(\mathbf{V}_{k}) = \mathcal{K}_{k}(\mathbf{A}, \mathbf{b})$$

= span{b, Ab, ..., A^{k-1}b}, (5)
$$COLSP(\mathbf{W}_{k}) = \mathcal{K}_{k}(\mathbf{A}^{T}, \mathbf{c}^{T})$$

$$= \operatorname{span}\{\mathbf{c}^{T}, \mathbf{A}^{T}\mathbf{c}^{T}, \dots, \mathbf{A}^{k-1}\mathbf{c}^{T}\}. (6)$$

The utility of selecting \mathbf{V}_k and \mathbf{W}_k in Krylov spaces comes from the fact that they can be generated with only innerproducts and matrix-vector multiplications, thereby allowing for the exploitation of the sparsity or structure of \mathbf{A} .

But regardless of how quickly π_k can be computed, one is certainly also interested in the correspondence between the original system $\{\mathbf{A}, \mathbf{b}, \mathbf{c}\}$ and the reduced-order system $\{\hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$. An important insight into this relationship comes from [11, 25].

Theorem 1 Let the reduced-order system $\{\hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$ be a restriction of the system $\{\mathbf{A}, \mathbf{b}, \mathbf{c}\}$ by the projector π_k where \mathbf{V}_k and \mathbf{W}_k are defined as in (5) and (6) respectively. Then the first 2k Markov parameters of the original and reduced-order systems are identical.

Restating Theorem 1, the reduced-order model is a Padé approximation (partial realization) which matches the first 2k high-frequency moments of the original system.

Through a projector corresponding to $\mathcal{K}_k(\mathbf{A}, \mathbf{b})$ and $\mathcal{K}_k(\mathbf{A}^T, \mathbf{c}^T)$, one can obtain a state space realization which

matches moments about $s_0 = \infty$. In a completely analogous manner, a projector corresponding to $\mathcal{K}_k(\mathbf{A}^{-1}, \mathbf{b})$ and $\mathcal{K}_k(\mathbf{A}^{-T}, \mathbf{c}^T)$ can be employed to generate a realization which matches moments about $s_0 = 0$ [25][†].

A popular technique for computing \mathbf{V}_k and \mathbf{W}_k in the Krylov projector is due to Lanczos [10, 17]. Given the starting vectors \mathbf{v}_1 and \mathbf{w}_1 , the Lanczos algorithm produces the rectangular matrices $\mathbf{V}_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k] \in \mathbf{R}^{n \times k}$ and $\mathbf{W}_k = [\mathbf{w}_1, \ldots, \mathbf{w}_k] \in \mathbf{R}^{n \times k}$ which satisfy the recursive identities

$$\mathbf{A}\mathbf{V}_{k} = \mathbf{V}_{k}\mathbf{T}_{k} + \beta_{k+1}\mathbf{v}_{k+1}\mathbf{e}_{k}^{T}, \qquad (7)$$

$$\mathbf{A}^T \mathbf{W}_k = \mathbf{W}_k \mathbf{T}_k^T + \gamma_{k+1} \mathbf{w}_{k+1} \mathbf{e}_k^T.$$
 (8)

The vector \mathbf{e}_k is the k^{th} standard basis vector while \mathbf{T}_k is a truncated reduction of \mathbf{A} that is in tridiagonal form. Generally, the elements β_i and γ_i are chosen so that $\mathbf{V}_{k+1}^T \mathbf{W}_{k+1} = \mathbf{I}$. When \mathbf{V}_{k+1} and \mathbf{W}_{k+1} are biorthogonal, multiplying (7) on the left by \mathbf{W}_k^T yields the relationship $\mathbf{W}_k^T \mathbf{A} \mathbf{V}_k = \mathbf{T}_k$.

To choose the starting vectors, \mathbf{v}_1 and \mathbf{w}_1 , it is important to note from (7) and (8) that $\mathbf{v}_{k+1} \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{v}_1)$ and $\mathbf{w}_{k+1} \in \mathcal{K}_{k+1}(\mathbf{A}^T, \mathbf{w}_1)$. Then if $\mathbf{v}_1 = \mathbf{b}/\beta_1$ and $\mathbf{w}_1 = \mathbf{c}^T/\gamma_1$, the matrices \mathbf{V}_k and \mathbf{W}_k correspond to the Krylov spaces $\mathcal{K}_k(\mathbf{A}, \mathbf{b})$ and $\mathcal{K}_k(\mathbf{A}^T, \mathbf{c}^T)$ respectively. And more importantly from (4), $\hat{\mathbf{A}} = \mathbf{W}_k^T \mathbf{A} \mathbf{V}_k = \mathbf{T}_k$, $\hat{\mathbf{b}} = \mathbf{W}^T \mathbf{b} = \mathbf{e}_1 \beta_1$ and $\hat{\mathbf{c}} = \mathbf{c} \mathbf{V}_k = \mathbf{e}_1^T \gamma_1$, which is our reduced-order model.

Compared to explicit moment matching, the Lanczos method provides superior results and/or greater flexibility in several areas [4, 7]. In particular, the remainder of this section demonstrates that the Lanczos method is able to successfully treat the first two Padé shortcomings listed in §1.

Note that explicitly computing moments entails a power method approach. If $s_0 = \infty$ for example, the product $\mathbf{A}^{j}\mathbf{b}$ must be computed for successively higher powers of j. But it is well known that the product $\mathbf{A}^{j}\mathbf{b}$ will converge to that eigenvector corresponding to the largest eigenvalue of A as j increases. In finite precision, the information corresponding to the other eigenvectors will be lost in the higher moments. The Hankel matrix, M, containing the moments will become nearly singular. And regardless of how many additional moments are supposedly matched in this situation, the computed approximation never converges to the original one (see [1, example 1]). To contend with this difficulty, [1] suggests working around the problem by attempting to modify the expansion frequency, s_0 . If forming a certain type of moment emphasizes an extreme eigenvalue of \mathbf{A} , one must select other types of moments which emphasize information from other portions of the spectrum.

The Lanczos method, on the other hand, completely avoids this issue because it never computes the moments. Rather $\{\hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$ are computed from Krylov spaces. Maintaining the biorthogonality \mathbf{V}_k and \mathbf{W}_k insures that additional information is introduced into the projection as kis incremented. As an example, consider the state space

[†]Although analogous in approach to the $s_0 = \infty$ case, the computation of the Krylov spaces corresponding to $s_0 = 0$ is more costly as a series of linear equations must be solved.

equations arising from a small, stiff RC ladder circuit

$$\begin{bmatrix} \mathbf{A} & \mathbf{b} \\ \hline \mathbf{c} & d \end{bmatrix} = \begin{bmatrix} -2C_1^{-1} & C_1^{-1} & 0 & C_1^{-1} \\ C_2^{-1} & -2C_2^{-1} & C_2^{-1} & 0 \\ 0 & C_3^{-1} & -C_3^{-1} & 0 \\ \hline 1 & -1 & 0 & 0 \end{bmatrix}$$

where $C_1 = 10^{-3}$, $C_2 = 10^{-6}$, and $C_3 = 10^{-9}$. Allowing k = 3, the eigenvalues of the realization obtained with both explicit moment matching (about $s_0 = 0$) and the Lanczos method (corresponding to $\mathcal{K}_k(\mathbf{A}^{-1}, \mathbf{b})$ and $\mathcal{K}_k(\mathbf{A}^{-T}, \mathbf{c}^T)$) are presented in Table 2. Due to the poor scaling of the moments, explicit moment matching is unable to accurately determine the fastest pole. The Lanczos method, on the other hand, can capture all of the eigenvalues, λ , of **A**.

Table 1: Computed Eigenvalues of A

	Exact	Explicit Match	Lanczos
λ_1	-9.98999000e2	$-9.89999000 \mathrm{e2}$	-9.98999000e2
λ_2	-1.00000100e6	-1.00000078e6	-1.00000100e6
λ_3	-1.00100100e9	-5.45486876e6	-1.00100100e9

Even if explicit moment matching can somehow avoid the loss of precision due to its power method approach, singularities can still occur in the moment matrix, M. Such singularities depend only on the properties of the system itself [18]. Where they exist, partial realizations (2) will not be possible. Additionally, nearly singular matrices must be avoided. This issue is oftentimes not addressed in explicit moment matching. Yet the occurrence of singularities is well-studied in the context of the Lanczos algorithm [13, 14], where it is termed a serious breakdown. By employing lookahead into the Lanczos method [6], one possesses a powerful tool for detecting and avoiding ill-conditioned entries in the Padé table.

3. Multi-point Padé approximation with Lanczos $\mathbf{methods}$

In this section, we extend the results and benefits of existing Lanczos methods to the case of generalized state space systems (i.e., $\mathbf{E} \neq \mathbf{I}$). This new technique possesses the additional advantage of allowing for multi-point Padé approximation. That is, the resulting reduced-order model of dimension $k = \bar{i}\bar{j}$ satisfies

$$m_j(s_i) = \hat{m}_j(s_i), \quad j = 1, 2, \dots, 2\bar{j}, \quad i = 1, 2, \dots, \bar{i}, \quad (9)$$

where

$$m_j(s_i) = \mathbf{c} \left\{ (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{E} \right\}^{j-1} (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{b}$$

is the j^{th} moment of (1) about the expansion frequency s_i and

$$\hat{m}_j(s_i) = \hat{\mathbf{c}} \left\{ (\hat{\mathbf{A}} - s_i \hat{\mathbf{E}})^{-1} \hat{\mathbf{E}} \right\}^{j-1} (\hat{\mathbf{A}} - s_i \hat{\mathbf{E}})^{-1} \hat{\mathbf{b}}$$

is the j^{th} moment of reduced-order model about s_i . It will be assumed for notational simplicity that $2\bar{j}$ moments are to be matched about each of the frequencies s_1 through s_i . In general, the number of moments matched may vary from expansion frequency to expansion frequency. One can easily modify the following results to handle this case.

The variant of the Lanczos method employed to generate a reduced-order model $\{\hat{\mathbf{E}}, \hat{\mathbf{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$ satisfying (9) will be denoted the rational Lanczos algorithm as it is an adaptation of the rational Arnoldi method of [20, 21]. The most glaring difference between the two rational methods is that rational Lanczos computes a biorthogonal \mathbf{V}_k and \mathbf{W}_k rather than an orthogonal \mathbf{V}_k . There are, however, smaller dissimilarities between the two methods which are necessary to insure that the oblique projector, $\pi = \mathbf{V}_k \mathbf{W}_k$, of rational Lanczos yields multi-point Padé approximants.

Algorithm 1 Rational Lanczos algorithm

Initialize $\mathbf{r}_0 = (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{b}$ and $\mathbf{q}_0 = \mathbf{c}^T$;

For i = 1 to \overline{i} ,

6

For
$$j = 1$$
 to \bar{j} ,
(1) $k = (i - 1)\bar{j} + j$;
(2) $h_{k,k-1} = \sqrt{|\mathbf{r}_{k-1}^T \mathbf{q}_{k-1}|}$
(3) $\mathbf{v}_k = (\mathbf{r}_{k-1}/h_{k,k-1})$ and
 $\mathbf{w}_k = sign(\mathbf{r}_{k-1}^T \mathbf{q}_{k-1}) \cdot (\mathbf{q}_{k-1}/h_{k,k-1})$;
(4) if $j < \bar{j}$ and $i < \bar{i}$,
(4.1) $\mathbf{r}_k = (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{E} \mathbf{v}_k$ and
 $\mathbf{q}_k = \mathbf{E}^T (\mathbf{A} - s_i \mathbf{E})^{-T} \mathbf{w}_k$;
else if $j = \bar{j}$ and $i < \bar{i}$,
(4.2) $\mathbf{r}_k = (\mathbf{A} - s_{i+1} \mathbf{E})^{-1} \mathbf{b}/h_{1,0}$ and
 $\mathbf{q}_k = \mathbf{E}^T (\mathbf{A} - s_{i+1} \mathbf{E})^{-T} \mathbf{c}^T$;
else
(4.3) $\mathbf{r}_k = (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{E} \mathbf{v}_{\bar{j}}$ and
 $\mathbf{q}_k = \mathbf{E}^T (\mathbf{A} - s_1 \mathbf{E})^{-T} \mathbf{w}_{\bar{j}}$;
end
(5) $h_{1...k,k} = \mathbf{W}_k^T \mathbf{r}_k$ and $g_{1...k,k} = \mathbf{V}_k^T \mathbf{q}_k$;
(6) $\mathbf{r}_k = \mathbf{r}_k - \mathbf{V}_k h_{1...k,k}$ and $\mathbf{q}_k = \mathbf{q}_k - \mathbf{W}_k g_{1...k,k}$
end
end

$$\mathbf{v}_{\bar{\imath}\bar{\jmath}+1} = (\mathbf{r}_{\bar{\imath}\bar{\jmath}}/h_{\bar{\imath}\bar{\jmath}+1,\bar{\imath}\bar{\jmath}}) \ where \ h_{\bar{\imath}\bar{\jmath}+1,\bar{\imath}\bar{\jmath}} = \sqrt{|\mathbf{r}_{\bar{\imath}\bar{\jmath}}^T \mathbf{q}_{\bar{\imath}\bar{\jmath}}|}.$$

Strong similarities exist between Algorithm 1 and the traditional Lanczos algorithm (see [10] for the standard method). The key difference between the standard and rational Lanczos algorithms lies in step (4) of Algorithm 1. In rational Lanczos the matrix, $(\mathbf{A} - s\mathbf{E})^{-1}\mathbf{E}$, multiplying the previous **v** vector changes with the expansion frequency. By making this matrix a function of s, sequences of Krylov spaces are computed.

Theorem 2 If \mathbf{V}_k and \mathbf{W}_k are the results of the first k steps of the rational Lanczos algorithm with $1 \leq k \leq \overline{ij}$ then

$$\operatorname{colsp}(\mathbf{V}_{k}) = \left\{ \mathcal{K}_{k-\overline{j}(i-1)} \left((\mathbf{A} - s_{i}\mathbf{E})^{-1}\mathbf{E}, (\mathbf{A} - s_{i}\mathbf{E})^{-1}\mathbf{b} \right) \\ \bigcup_{l=1}^{i-1} \mathcal{K}_{\overline{j}} \left((\mathbf{A} - s_{l}\mathbf{E})^{-1}\mathbf{E}, (\mathbf{A} - s_{l}\mathbf{E})^{-1}\mathbf{b} \right) \right\}$$

$$\operatorname{colsp}(\mathbf{W}_{k}) = \left\{ \mathcal{K}_{\bar{\jmath}} \left(\mathbf{E}^{T} (\mathbf{A} - s_{1} \mathbf{E})^{-T}, \mathbf{c}^{T} \right) \\ \bigcup_{l=2}^{i-1} \mathcal{K}_{\bar{\jmath}} \left(\mathbf{E}^{T} (\mathbf{A} - s_{l} \mathbf{E})^{-T}, \mathbf{E}^{T} (\mathbf{A} - s_{l} \mathbf{E})^{-T} \mathbf{c}^{T} \right) \\ \bigcup \mathcal{K}_{k-\bar{\jmath}(i-1)} \left(\mathbf{E}^{T} (\mathbf{A} - s_{i} \mathbf{E})^{-T}, \mathbf{E}^{T} (\mathbf{A} - s_{i} \mathbf{E})^{-T} \mathbf{c}^{T} \right) \right\}$$

if i > 1; otherwise

$$\operatorname{colsp}(\mathbf{W}_k) = \mathcal{K}_k \left(\mathbf{E}^T (\mathbf{A} - s_1 \mathbf{E})^{-T}, \mathbf{c}^T \right).$$

Proof: Due to space constraints we refer the reader to [8].

Recall that the \mathbf{V}_k and \mathbf{W}_k matrices resulting from the standard Lanczos method each corresponded to a single Krylov space. In the rational Lanczos method, multiple Krylov spaces are computed. Each space corresponds to an expansion frequency s_i . The cost of combining multiple Krylov spaces into \mathbf{V}_k and \mathbf{W}_k is the loss of a three-term recurrence in step (6) of the algorithm. Thus one should expect to see upper-Hessenberg rather than tridiagonal matrices appearing out of the rational Krylov projection.

As one is ultimately interested in obtaining a rational Krylov projection of (1), the effects of \mathbf{V}_k and \mathbf{W}_k on \mathbf{A} and \mathbf{E} are of interest. To obtain a relationship between \mathbf{V}_k , \mathbf{W}_k , \mathbf{A} and \mathbf{E} , we begin by analyzing Algorithm 1 for the case when k is a multiple of \bar{j} . This case involves the execution of step (4.2) and corresponds to a change in the expansion frequency from s_i to s_{i+1} . Note that $h_{k+1,k} \mathbf{v}_{k+1} = \mathbf{r}_k$ due to step (3). Then plugging step (4.2) into step (6)'s expression for \mathbf{r}_k yields

$$\mathbf{V}_{k+1} \begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \end{bmatrix} = h_{1,0}^{-1} (\mathbf{A} - s_{i+1} \mathbf{E})^{-1} b$$
$$= (\mathbf{A} - s_{i+1} \mathbf{E})^{-1} (\mathbf{A} - s_1 \mathbf{E}) \mathbf{V}_k \mathbf{e}_1$$
(10)

since $h_{1,0}\mathbf{v}_1 = (\mathbf{A} - s_1 \mathbf{E})^{-1}\mathbf{b}$. Multiplying (10) on the right by $(\mathbf{A} - s_{i+1}\mathbf{E})$ and rearranging the expression results in

$$\mathbf{AV}_{k+1} \left(\begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \end{bmatrix} - \begin{bmatrix} \mathbf{e}_1 \\ 0 \end{bmatrix} \right) = \mathbf{EV}_{k+1} \left(s_{i+1} \begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \end{bmatrix} - s_1 \begin{bmatrix} \mathbf{e}_1 \\ 0 \end{bmatrix} \right)$$

which can be rewritten as

$$(\mathbf{A} - s_1 \mathbf{E}) \mathbf{V}_{\mathbf{r}\mathbf{j}+1} \underbrace{\left(\begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \\ 0 \end{bmatrix} - \begin{bmatrix} \mathbf{e}_1 \\ 0 \\ 0 \end{bmatrix} \right)}_{\mathbf{h}_k} = \mathbf{E} \mathbf{V}_{\mathbf{r}\mathbf{j}+1} \underbrace{\left(\begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \\ 0 \end{bmatrix} (s_{i+1} - s_1) \right)}_{\mathbf{k}_k}.$$
(11)

When k is not a multiple of \bar{j} , step (4.1) is executed and the next **v** vector computed is still associated with the expansion frequency s_i . For this case, placing step (4.1) into step (6)'s expression for \mathbf{r}_k yields

$$\mathbf{V}_{k+1} \begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \end{bmatrix} = (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{E} \mathbf{V}_k \mathbf{e}_k.$$
(12)

Multiplying (12) on the left by $(\mathbf{A} - s_i \mathbf{E})$ produces

$$\mathbf{E}\mathbf{V}_{k}\mathbf{e}_{k} = (\mathbf{A} - s_{i}\mathbf{E})\mathbf{V}_{k+1} \begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \end{bmatrix}$$

which can be rewritten as

$$(\mathbf{A} - s_{1}\mathbf{E})\mathbf{V}_{ij+1}\underbrace{\begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \\ 0 \end{bmatrix}}_{\mathbf{h}_{k}} = \mathbf{E}\mathbf{V}_{ij+1}\underbrace{\left(\begin{bmatrix} h_{1\dots k,k} \\ h_{k+1,k} \\ 0 \end{bmatrix} (s_{i} - s_{1}) + \begin{bmatrix} \mathbf{e}_{k} \\ 0 \\ 0 \end{bmatrix}\right)}_{\mathbf{k}_{k}}.$$
(13)

Combining all $\bar{k} \equiv \bar{i}\bar{j}$ steps of Algorithm 1 yields

$$(\mathbf{A} - s_1 \mathbf{E}) \mathbf{V}_{\bar{k}+1} \mathbf{H}_{\bar{k}+1,\bar{k}} = \mathbf{E} \mathbf{V}_{\bar{k}+1} \mathbf{K}_{\bar{k}+1,\bar{k}}$$
(14)

where the columns of $\mathbf{H}_{\bar{k}+1,\bar{k}}$ and $\mathbf{K}_{\bar{k}+1,\bar{k}}$ are defined via (11) and (13). Specifically, columns $\bar{j}, 2\bar{j}, \ldots, (\bar{i}-1)\bar{j}$ of $\mathbf{H}_{\bar{k}+1,\bar{k}}$ and $\mathbf{K}_{\bar{k}+1,\bar{k}}$ fit the form of (11) while the remaining columns satisfy (13). Note that $\mathbf{H}_{\bar{k}+1,\bar{k}}$ and $\mathbf{K}_{\bar{k}+1,\bar{k}}$ are upper-Hessenberg. Special mention should also be given to the \bar{k}^{th} columns of $\mathbf{H}_{\bar{k}+1,\bar{k}}$ and $\mathbf{K}_{\bar{k}+1,\bar{k}}$. Due to step (4.3) of Algorithm 1, the \bar{k}^{th} column satisfies the general form of (13) with $s_i = s_1$. Thus $\mathbf{k}_{\bar{k}} = [\mathbf{e}_{\bar{j}}^T \ \mathbf{0}]^T$ so that $\mathbf{V}_{\bar{k}+1}\mathbf{K}_{\bar{k}+1,\bar{k}} = \mathbf{V}_{\bar{k}}\mathbf{K}_{\bar{k},\bar{k}}$. Making use of this last fact when multiplying (14) on the left by $\mathbf{W}_{\bar{k}}^T(\mathbf{A} - s_1\mathbf{E})^{-1}$ yields

$$\mathbf{H}_{\tilde{k},\tilde{k}} = \mathbf{W}_{\tilde{k}}^{T} (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{E} \mathbf{V}_{\tilde{k}} \mathbf{K}_{\tilde{k},\tilde{k}}.$$
 (15)

Expressions (14) and (15) serve as the principal relations between the projector $\mathbf{V}_{\bar{k}} \mathbf{W}_{\bar{k}}^T$ and \mathbf{E} and \mathbf{A} .

For the remainder of this section, it will be assumed that Algorithm 1 is executed to completion and the value of k will be fixed as $k = \bar{k} \equiv \bar{\imath}\bar{\jmath}$. Then given the results of the rational Lanczos method, we will define the reduced-order model so that

$$\hat{\mathbf{A}} = \mathbf{K}_{k,k} + s_1 \mathbf{H}_{k,k}, \qquad \qquad \hat{\mathbf{E}} = \mathbf{H}_{k,k},$$

$$\hat{\mathbf{b}} = \mathbf{W}_k^T (\mathbf{A} - s_1 \mathbf{E})^{-1} b, \qquad \qquad \hat{\mathbf{c}} = \mathbf{c} \mathbf{V}_k \mathbf{K}_{k,k}.$$
(16)

To begin to motivate the choices in (16), rewrite the definition (1) of the original system as

$$\begin{cases} (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{E} \dot{\mathbf{x}} = \\ (\mathbf{A} - s_1 \mathbf{E})^{-1} (\mathbf{A} - s_1 \mathbf{E} + s_1 \mathbf{E}) \mathbf{x} + (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{b} u \\ y = \mathbf{c} \mathbf{x}. \end{cases}$$

The restriction of the original system by the projector π is formed by replacing the state vector, \mathbf{x} , with $\mathbf{V}_k \mathbf{W}_k^T \mathbf{x}$ and multiplying on the left by \mathbf{W}_k^T to yield

$$\begin{cases} \mathbf{W}_{k}^{T} (\mathbf{A} - s_{1} \mathbf{E})^{-1} E \pi \dot{\mathbf{x}} = \\ \mathbf{W}_{k}^{T} \mathbf{x} + s_{1} \mathbf{W}_{k}^{T} (\mathbf{A} - s_{1} \mathbf{E})^{-1} E \pi \mathbf{x} + \\ \mathbf{W}_{k}^{T} (\mathbf{A} - s_{1} \mathbf{E})^{-1} \mathbf{b} u \\ \hat{y} = \mathbf{c} \mathbf{V}_{k} \mathbf{W}_{k}^{T} \mathbf{x}. \end{cases}$$
(17)

If one *temporarily* assumes that $\mathbf{K}_{k,k}$ is invertible, (15) can be used to rewrite (17) as

$$\begin{pmatrix} \mathbf{H}_{k,k} \mathbf{K}_{k,k}^{-1} \mathbf{W}_{k}^{T} \dot{\mathbf{x}} = \\ s_{1} \mathbf{H}_{k,k} \mathbf{K}_{k,k}^{-1} \mathbf{W}_{k}^{T} \mathbf{x} + \mathbf{W}_{k}^{T} \mathbf{x} + \mathbf{W}_{k}^{T} (\mathbf{A} - s_{1} \mathbf{E})^{-1} \mathbf{b} u \\ \hat{y} = \mathbf{c} \mathbf{V}_{k} \mathbf{W}_{k}^{T} \mathbf{x}. \end{cases}$$

which in turn becomes

$$\begin{cases} \mathbf{H}_{k,k} \dot{\mathbf{x}} = \\ (\mathbf{K}_{k,k} + s_1 \mathbf{H}_{k,k}) \hat{\mathbf{x}} + \mathbf{W}_k^T (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{b}u \qquad (18) \\ \hat{y} = \mathbf{c} \mathbf{V}_k \mathbf{K}_{k,k} \hat{\mathbf{x}}. \end{cases}$$

by defining $\hat{\mathbf{x}}(t)$ to be $\mathbf{K}_{k,k}^{-1} \mathbf{W}_k^T \mathbf{x}(t)$.

Comparing (2) and (18) indicates that the prescribed choices for $\hat{\mathbf{A}}$, $\hat{\mathbf{E}}$, $\hat{\mathbf{b}}$ and $\hat{\mathbf{c}}$ are quite logical. However, (18) was obtained assuming $\mathbf{K}_{k,k}$ to be invertible. This assumption is in fact not necessary for our purposes. The following result states that the reduced-order model corresponding to (16) matches the desired moments of the original system without placing any restrictions on the invertibility of $\mathbf{K}_{k,k}$ or \mathbf{E} .

Theorem 3 Let the jth moments of the original and reduced order systems about the expansion frequency s_i be $m_j(s_i) = \mathbf{c} \{ (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{E} \}^{j-1} (\mathbf{A} - s_i \mathbf{E})^{-1} \mathbf{b}$ and $\hat{m}_j(s_i) = \hat{\mathbf{c}} \{ (\hat{\mathbf{A}} - s_i \hat{\mathbf{E}})^{-1} \hat{\mathbf{E}} \}^{j-1} (\hat{\mathbf{A}} - s_i \hat{\mathbf{E}})^{-1} \hat{\mathbf{b}}$ respectively. If $\hat{\mathbf{A}} = \mathbf{K}_{k,k} + s_1 \mathbf{H}_{k,k}$, $\hat{\mathbf{E}} = \mathbf{H}_{k,k}$, $\hat{\mathbf{b}} = \mathbf{W}_k^T (\mathbf{A} - s_1 \mathbf{E})^{-1} \mathbf{b}$ and $\hat{\mathbf{c}} = \mathbf{c} \mathbf{V}_k \mathbf{K}_{k,k}$ where $\mathbf{H}_{k+1,k}$, $\mathbf{K}_{k+1,k}$, \mathbf{V}_{k+1} and \mathbf{W}_{k+1} are the results of Algorithm 1 with $k = \bar{\imath}\bar{\jmath}$, then $m_j(s_i) = \hat{m}_j(s_i)$ for $i = 1, 2, \ldots, \bar{\imath}$ and $j = 1, 2, \ldots, 2\bar{\jmath}$.

Proof: see [8].

Thus the projection resulting from the rational Lanczos method satisfies the multi-point condition of (9). It also would appear that the benefits of the standard Lanczos method (e.g., avoiding a power method, look-ahead) can be easily extended to the rational Lanczos approach.

4. Example

As a brief example of the utility of multi-point Padé approximations, we will study the 120^{th} order system which describes the effects of a magnetic actuator on the radial tracking arm of a portable compact disc player, see [12]. Figure 1 plots the frequency responses of the original system (solid line), a 24^{th} order Padé approximation about $s_0 = \infty$ (dashed line), a 12^{th} order Padé approximation about $s_0 = 0$ (dotted line) and a 6^{th} order multi-point Padé approximation (dashed-dotted line) for the CD player. The multi-point approximation matches six moments expanded about $s_1 = 0$, four moments about $s_2 = 10^5$, and two moments about $s_3 = 10^4$. To keep this example short, a discus-

sion of the algorithm used to choose these expansion points must be postponed until a later time.



Figure 1: Frequency responses for the example.

Note that the frequency response of the original system displays two sharp peaks at $w \approx 30$ and $w \approx 30^4$. The frequency response of the multi-point Padé approximation captures both of these peaks and is almost indistinguishable with the response of the original system. As one should expect, the Padé approximation about $s_0 = 0$ displays the first peak but demonstrates significant error at high frequencies. The approximation about infinity, on the other hand, captures the second peak but smoothes over the peak at $w \approx 30$.

The impulse response of the stable, original system is dominated by those modes corresponding to the frequency response peak at $w \approx 30$. The multi-point approximation is stable and its impulse response recreates that of the original system with great precision. The Padé approximation about $s_0 = 0$ identifies those modes corresponding to the low-frequency peak but its impulse response is unstable. However, the techniques of [12] can stabilize the $s_0 = 0$ approximation so that the $s_0 = 0$ response to an impulse (which may or may not be the input of interest for a given application) follows that of the original system with great precision. Finally, the Padé approximation about infinity is not stable nor does it capture those modes corresponding to the low-frequency peak. As a result, even a stabilized model about $s_0 = \infty$ does a poor job of approximating the system's impulse response. Note that because the Krylov sequences corresponding to $s_0 = \infty$ do not invert A, the oftentimes desirable low-frequency information is lost.

5. Conclusion

Both explicit moment matching and the Lanczos algorithm are efficient techniques for generating partial realizations of large-scale systems. But by either avoiding a difficulty or providing well-defined techniques for fixing it, the Lanczos method is better suited for handling the problems inherent to Padé approximation. Through Algorithm 1, the Lanczos method can be extended to treat multiple expansion frequencies. Multipoint approximation shows promise in several applications [16, 19, 26] as an approach for handling false instabilities and frequency response errors in the reduced-order model. However, the techniques for choosing the expansion frequencies are still rather heuristic; a more formal approach should be explored in future work.

The Lanczos method must also still be extended to the multiple input-multiple output (MIMO) case. Block versions of the Lanczos method are already in existence, see [2] for example. But the extension of look-ahead to handle the breakdowns in MIMO Lanczos remains an open issue.

Finally, we note that the inversion of $(\mathbf{A} - s_i \mathbf{E})$ is an area requiring additional work. Regardless of whether explicit moment matching or the Lanczos method is being employed, one must avoid explicit inversions and instead utilize sparse factorizations of the matrix or iterative techniques. One must further insure that the values for s_i are chosen so that $(\mathbf{A} - s_i \mathbf{E})$ is well-conditioned.

6. References

- M. M. Alaybeyi, J. Y. Lee and R. A. Rohrer, "Numerical integration algorithms and asymptotic waveform evaluation (AWE)," *Tech. Digest IEEE Internat. Conf. on Computer-Aided Design*, 1992.
- [2] D. L. Boley, "Krylov space methods on state-space control models," Technical Report, Univ. of Minnesota, Minneapolis, MN 55455, 1992.
- [3] C. I. Byrnes and A. Lindquist, "The stability and instability of partial realizations," Systems Control Lett., vol. 2, pp. 99-105, 1982.
- [4] P. Feldman and R. W. Freund, "Efficient linear circuit analysis by Padé approximation via the Lanczos process," Technical Report, AT&T Bell Laboratories, Murray Hill, NJ 07974, 1994.
- [5] L. Fortuna, G. Nunnari and A. Gallo, Model Reduction Techniques with Applications in Electrical Engineering, London: Springer-Verlag, 1992.
- [6] R. W. Freund, M. H. Gutknecht and N. M. Nachtigal, "An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices," Technical Reports 90.45 and 90.46, RIACS, NASA Ames Research Center, 1990.
- [7] K. Gallivan, E. Grimme and P. Van Dooren, "Asymptotic waveform evaluation via a Lanczos method," to appear Appl. Math. Lett., 1994.
- [8] K. Gallivan, E. Grimme and P. Van Dooren, "Multipoint Padé approximation of large-scale systems via a two-sided rational Krylov algorithm," Techical Report, Univ. of Illinois, Urbana, IL 61801, 1994.
- [9] E. Gallopoulos and Y. Saad, "Efficient solution of parabolic equations by Krylov approximation methods," SIAM J. Sci. Statist. Comput., vol. 13, pp. 1236-1264, 1992.
- [10] G. H. Golub and C. Van Loan, Matrix Computations, 2nd ed. Baltimore, MD: Johns Hopkins University Press, 1989.

- [11] W. B. Gragg and A. Lindquist, "On the partial realization problem," *Linear Algebra and Appl.*, vol. 50, pp. 277-319, 1983.
- [12] E. Grimme, D. Sorensen and P. Van Dooren, "Model reduction of state space systems via an implicitly restarted Lanczos method," to appear Numer. Algorithms, 1994.
- [13] M. H. Gutknecht, "A completed theory of the unsymmetric Lanczos process and related algorithms: part I," SIAM J. Matrix Anal. Appl., vol. 13, pp. 594-639, 1992.
- [14] M. H. Gutknecht, "A completed theory of the unsymmetric Lanczos processes and related algorithms: part II," SIAM J. Matrix Anal. Appl., vol. 15, pp. 15-58, 1994.
- [15] I. M. Jaimoukha and E. M. Kasenally, "Oblique projection methods for large scale model reduction," to appear SIAM J. Matrix Anal. Appl., 1994.
- [16] C. Kenney, A. J. Laub and S. Stubberud, "Frequency response computation via rational interpolation," *IEEE Trans. Automatic Control*, vol. AC-38, pp. 1203-1213, 1993.
- [17] C. Lanczos, "An iteration method for the solution of the eigenvalue problem of linear differential and integral operators," J. Res. Nat. Bureau Stan., vol. 45, pp. 255-282, 1950.
- [18] B. N. Parlett, "Reduction to tridiagonal form and minimal realizations," SIAM J. Matrix Anal. Appl., vol. 13, pp. 567-593, 1992.
- [19] V. Raghavan, R. A. Rohrer, L. T. Pillage, J. Y. Lee, J. E. Bracken and M. M. Alaybeyi, "AWE-Inspired," *Proc. of the IEEE Custom Integrated Circuits Conf.*, 1993.
- [20] A. Ruhe, "Rational Krylov algorithms for nonsymmetric eigenvalue problems, II: Matrix pairs," *Linear Al*gebra and Appl., vol. 194, 1993.
- [21] A. Ruhe, "The rational Krylov algorithm for nonsymmetric eigenvalue problems, III: Complex shifts for real matrices," *BIT*, vol. 34, 1994.
- [22] Y. Saad, "Analysis of some Krylov subspace approximations to the matrix exponential operator," SIAM J. Numer. Anal., vol. 29, pp. 209-228, 1992.
- [23] T. J. Su and R. R. Craig Jr., "An unsymmetric Lanczos algorithm for damped structural dynamics systems," *Proc. 33rd Conf. on Structures, Structural Dynamics* and Materials, 1992.
- [24] P. Van Dooren, "Numerical linear algebra techniques for large scale matrix problems in systems and control," *Proc. 31st IEEE Conf. on Decision and Control*, (Tucson, AZ), 1992.
- [25] C. D. Villemagne and R. E. Skelton, "Model reduction using a projection formulation," *Internat. J. Control*, vol. 46, pp. 2141-2169, 1987.
- [26] H. Xiheng, "FF-Padé method of model reduction in frequency domain," *IEEE Trans. Automatic Control*, vol. AC-32, pp. 243-246, 1987.