Adaptive rational Krylov algorithms for model reduction

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Abstract— **The Arnoldi and Lanczos algorithms, which belong to the class of Krylov subspace methods, are increasingly used for model reduction of large scale systems. The standard versions of the algorithms tend to create reduced order models that poorly approximate low frequency dynamics. Rational Arnoldi and Lanczos algorithms produce reduced models that approximate dynamics at various frequencies. This paper tackles the issue of developing simple Arnoldi and Lanczos equations for the rational case that allow simple residual error expressions to be derived. This in turn permits the development of computationally efficient model reduction algorithms, where the frequencies at which the dynamics are to be matched can be updated adaptively resulting in an optimized reduced model.**

I. Introduction

Consider a linear time-invariant single-input single-output system described by the state-space equations

$$E\dot{x}(t) = Ax(t) + Bu(t), \qquad y(t) = Cx(t) \qquad (1)$$

where $x(t) \in \mathcal{C}^n$ denotes the state vector and $u(t)$ and $y(t)$ the scalar input and output signals, respectively. The system matrices $A,\ E \in \mathcal{C}^{n\times n}$ are assumed to be large and sparse, and $B,\ C' \in \mathcal{C}^n$. These assumptions are met by large scale models in many applications. The transfer function for the system in (1) is denoted as

$$G(s) = C(sE-A)^{-1}B \stackrel{s}{=} \left[\begin{array}{cc|c} E & A & B \\ \hline * & C & 0 \end{array}\right].$$

To simplify subsequent analysis and design based on the large nth order model in (1), the model reduction problem seeks an approximate mth order model of the form

$$E_m\dot{x}_m(t) = A_m x_m(t) + B_m u(t), \qquad y_m(t) = C_m x_m(t)$$

where $x_m(t) \in \mathcal{C}^m,\ E_m,\ A_m \in \mathcal{C}^{n\times m},\ B_m,\ C_m' \in \mathcal{C}^m$ and $m < n$. The associated lower order transfer function is denoted by

$$G_m(s) = C_m(sE_m-A_m)^{-1}B_m \stackrel{s}{=} \left[\begin{array}{cc|c} E_m & A_m & B_m \\ \hline * & C_m & 0 \end{array}\right].$$

Krylov projection methods, and in particular Arnoldi and Lanczos algorithms [1]–[5], have been extensively used for model reduction of large scale systems; see [5]–[8] and the references therein. Methods related to the work of [9], [10] use Krylov subspace methods to obtain bases for the controllability and observability subspaces; projecting the original system using these bases results in a reduced system that matches the transfer function and the derivatives of the transfer function of the system evaluated around infinity. The advantage associated to the projection methods using the bases of the controllability and observability subspaces is the existence of a set of equations known as the standard Arnoldi and Lanczos equations. The Arnoldi and Lanczos equations can be used to derive algorithms based on the standard Arnoldi and Lanczos algorithms, which improve further the approximations. Implicit restarts are an example [11]. Moreover the specific form of the standard equations allows the use of Arnoldi and Lanczos methods directly for solving large Lyapunov equations; see [10], [12]. Another important benefit associated to the standard Arnoldi and Lanczos equations is that simple residual error expressions can be derived through them, which provide useful stopping criteria for the algorithms.

Unfortunately the standard versions of the Arnoldi and Lanczos algorithms tend to create reduced order models that poorly approximated low frequency dynamics. Rational Arnoldi and Lanczos algorithms [13]–[16] are Krylov projection methods which produce reduced models that approximate the dynamics of the system at given frequencies. An existing research problem for the rational case is the efficient and fast selection of the interpolation frequencies to be matched. Such a task requires simple residual expressions and simple equations to describe these algorithms. A drawback of rational methods is that no simple Arnoldi and Lanczos-like equations exist. [14], [15], [17], [18] deal with these challenging problems where they give equations that describe the rational algorithms; however these equations are not in the standard Arnoldi and Lanczos form. The work of this paper studies the same problems but it is based on the development of Arnoldi and Lanczos-like equations for the rational case in the standard form. Residual error expressions can then be derived as in the case of standard Arnoldi and Lanczos methods and adaptive algorithms are developed.

The paper is organized as follows. Section II briefly describes the approximation problem by moment matching. The standard Lanczos and the rational Lanczos algorithms for moment matching are also described in this section. Section III gives the derivation of the Lanczos and Arnoldi-like equations and of the residual errors for the rational case. Section IV suggests new procedures for the efficient computation of the interpolation frequencies to improve the approximation and it gives the pseudo-code for the adaptive algorithm developed in this paper. Numerical results to illustrate the adaptive method are also presented and compared with the results of the standard rational method for model reduction and the results of balanced truncation. Finally

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section V gives our conclusions.

II. Moment matching problem

To simplify the presentation of our results, we only consider the case when $E = I_n$ where I_n is the identity matrix and we will write

$$G(s) = C(sI_n - A)^{-1}B \stackrel{s}{=} \left[\begin{array}{c|c} A & B \\ \hline C & 0 \end{array}\right].$$

The system in (1) can be expanded by Taylor series around an interpolation point $s_0 \in \mathcal{C}$ as

$$G(s) = \mu_0 + \mu_1(s - s_0) + \mu_2(s - s_0)^2 + \cdots$$

where the Taylor coefficients μ_i are known as the moments of the system around s_0 and are related to the transfer function of the system and its derivatives evaluated at s_0. The approximation problem by moment matching is to find a lower order system G_m with transfer function expanded as

$$G_m(s) = \hat{\mu}_0 + \hat{\mu}_1(s - s_0) + \hat{\mu}_2(s - s_0)^2 + \cdots$$

such that $\mu_i = \hat{\mu}_i$, for $i = 0, 1, \ldots, m$.

In the case where $s_0 = \infty$ the moments are called Markov parameters and are given by $\mu_i = CA^iB$. The moments around an arbitrary interpolation point $s_0 \in \mathcal{C}$ are known as shifted moments and they are defined as $\mu_i = C(s_0I_n - A)^{-(i+1)}B,\ i = 0, 1, \ldots$

A more general definition of approximation by moment matching is related to rational interpolation. By rational interpolation we mean that the reduced order system matches the moments of the original system at multiple interpolation points.

Let $V_m,\ W_m \in \mathcal{C}^{n\times m}$. By projecting the states of the high order system with the projector

$$P_m = V_m(W_m'V_m)^{-1}W_m', \tag{2}$$

assuming that $W_m'V_m$ is nonsingular, a reduced order model is obtained as:

$$\begin{aligned} G_m(s) &\stackrel{s}{=} \left[\begin{array}{cc|c} E_m & A_m & B_m \\ \hline * & C_m & 0 \end{array}\right] \\ &:= \left[\begin{array}{cc|c} W_m'V_m & W_m'AV_m & W_m'B \\ \hline * & CV_m & 0 \end{array}\right]. \end{aligned} \tag{3}$$

A careful selection of V_m and W_m as the bases of certain Krylov subspaces results in moment matching. For $R \in \mathcal{C}^{n\times n}$ and $Q \in \mathcal{C}^{n\times p}$ a Krylov subspace $\mathcal{K}_m(R, Q)$ is defined as

$$\mathcal{K}_m(R, Q) = \text{span}\left(\begin{bmatrix} Q & RQ & R^2Q & \cdots & R^{m-1}Q \end{bmatrix}\right).$$

If $m = 0$, $\mathcal{K}_m(R, Q)$ is defined to be the empty set.

A. Standard Lanczos algorithm

An iterative method for model reduction based on Krylov projections is the Lanczos process. The Lanczos process, given in algorithm 1, constructs the bases $V_m = [\,v_1, \ldots, v_m\,] \in \mathcal{C}^{n\times m}$ and $W_m = [\,w_1, \ldots, w_m\,] \in \mathcal{C}^{n\times m}$ for the Krylov sybspaces $\mathcal{K}_m(A, B)$ and $\mathcal{K}_m(A', C')$ respectively, such that they are biorthogonal, i.e., $W_m'V_m = I_m$.

The following equations, referred to as the Lanczos equations [19] hold,

$$\begin{aligned} AV_m &= V_mA_m + v_{m+1}C_{V_m} \\ B &= V_mB_m \\ A'W_m &= W_mA_m' + w_{m+1}B_{W_m}' \\ C &= C_mW_m'. \end{aligned}$$

Due to biorthogonality $W_{m+1}'V_{m+1} = I_{m+1}$, $W_m'v_{m+1} = V_m'w_{m+1} = 0$, the matrix A_m is in the tridiagonal form

$$A_m = \begin{bmatrix} \alpha_{11} & \alpha_{12} & & \\ \alpha_{21} & \alpha_{22} & \ddots & \\ & \ddots & \ddots & \alpha_{m-1,m} \\ & & \alpha_{m,m-1} & \alpha_{m,m} \end{bmatrix},$$

and

$$\begin{aligned} C_{V_m} &= w_{m+1}'AV_m = \alpha_{m+1,m}e_m^T \\ B_{W_m} &= v_{m+1}'A'W_m = \alpha_{m,m+1}'e_m^T \end{aligned}$$

The bases V_m and W_m are constructed such that $\mathcal{K}_m(A, B) \subseteq \text{colsp}(V_m)$ and $\mathcal{K}_m(A', C') \subseteq \text{colsp}(W_m)$ and so the reduced order system $G_m(s)$, defined in (3), matches the first $2m$ markov parameters of $G(s)$ [17].

B. Approximation and residual error expressions

The approximation error $\epsilon(s) = G(s) - G_m(s)$ in Krylov projection methods can be shown to be

$$\epsilon(s) = R_C(s)'(sI_n - A)^{-1}R_B(s), \tag{4}$$

where $R_C(s)$ and $R_B(s)$ are known as the residual errors. These are given by

$$\begin{aligned} R_B(s) &= B - (sI_n - A)V_mX_m(s), \\ R_C(s) &= C' - (sI_n - A)'W_mY_m(s). \end{aligned}$$

where $Y_m(s)$ and $X_m(s)$ are the solutions of the system of equations

$$\begin{aligned} (sI_m - A_m)X_m(s) &= B_m, \\ (sI_m - A_m)'Y_m(s) &= C_m', \end{aligned} \tag{5}$$

and satisfy the Petrov-Galerkin conditions

$$\begin{aligned} R_B(s) &\perp \text{span}\{W_m\}, \\ R_C(s) &\perp \text{span}\{V_m\}. \end{aligned}$$

i.e., $W_m'R_B(s) = V_m'R_C(s) = 0$. Using the Lanczos equations, the residual errors can be simplified as

$$R_B(s) = v_{m+1}C_{V_m}(sI_m - A_m)^{-1}B_m \tag{6}$$

$$R_C(s) = w_{m+1}B_{W_m}'(sI_m - A_m')^{-1}C_m' \tag{7}$$

which involves terms related to the reduced order system only.

Algorithm 1 Basic Lanczos algorithm

Inputs: A, B, C, m, ϵ
Initialize: $v_0 = 0$, $w_0 = 0$, $\hat{v}_1 = B$,$\hat{w}_1 = C'$
If $\{\sqrt{|\hat{w}_1'\hat{v}_1|} < \epsilon\}$, Stop **End**
$v_1 = \frac{\hat{v}_1}{\sqrt{|\hat{w}_1'\hat{v}_1|}}, \quad w_1 = \hat{w}_1 / \frac{\hat{w}_1'\hat{v}_1}{\sqrt{|\hat{w}_1'\hat{v}_1|}}$
for $j = 1$ *to* m
  $\alpha_{j,j} = w_j' A v_j, \qquad \alpha_{j-1,j} = w_{j-1}' A v_j,$
  $\alpha_{j,j-1} = w_j' A v_{j-1}$
  $\hat{v}_{j+1} = A v_j - v_{j-1}\alpha_{j-1,j} - v_j \alpha_{j,j}$
  $\hat{w}_{j+1} = A' w_j - w_{j-1}\alpha_{j,j-1}' - w_j \alpha_{j,j}'$
  $\alpha_{j+1,j} = \sqrt{|\hat{w}_{j+1}'\hat{v}_{j+1}|}$
  If $\{\alpha_{j+1,j} < \epsilon\}$, Stop **End**
  $\alpha_{j,j+1}' = \frac{\hat{w}_{j+1}'\hat{v}_{j+1}}{\alpha_{j+1,j}}$
  $v_{j+1} = \hat{v}_{j+1}/\alpha_{j+1,j}, \quad w_{j+1} = \hat{w}_{j+1}/\alpha_{j,j+1}'$
end
Outputs: $V_m = \{v_1, \ldots, v_m\}$,$W_m = \{w_1, \ldots, w_m\}$

C. The rational Lanczos method

The rational Lanczos procedure [14]–[16] is an algorithm for constructing biorthogonal bases of the union of Krylov subspaces. Let $V_m, W_m \in \mathcal{C}^{n \times m}$ be the bases of such subspaces and let P be a projector defined as $P = V_m W_m'$. Applying this projector on the system in (1) a reduced order system is obtained with a transfer function as in (3). The next result shows that a proper selection of Krylov subspaces will result in reduced order systems that matches the moments of the system at given interpolation frequencies.

Theorem 1: Let $\mathcal{S} = \{s_1, s_2, \ldots, s_K\}$ and $\tilde{\mathcal{S}} = \{\tilde{s}_1, \tilde{s}_2, \ldots, \tilde{s}_{\tilde{K}}\}$ be two sets of interpolation points. If

$$\bigcup_{k=1}^{K} \mathcal{K}_{m_{s_k}}((s_k I_n - A)^{-1}, (s_k I_n - A)^{-1} B) \subseteq \text{span}\{V_m\}$$

and

$$\bigcup_{k=1}^{\tilde{K}} \mathcal{K}_{m_{\tilde{s}_k}}((\tilde{s}_k' I_n - A')^{-1}, (\tilde{s}_k' I_n - A')^{-1} C') \subseteq \text{span}\{W_m\}$$

where m_{s_k} and $\tilde{m}_{\tilde{s}_k}$ are the multiplicities of the interpolation points s_k and $\tilde{s}_k$ respectively and $\sum_{k=1}^{K} m_{s_k} = \sum_{k=1}^{\tilde{K}} \tilde{m}_{\tilde{s}_k} = m$ then :

- if $s_k = \tilde{s}_k$ the reduced order system matches the first $m_{s_k} + \tilde{m}_{\tilde{s}_k}$ shifted moments around the interpolation point
- if $s_k \neq \tilde{s}_k$ the reduced order system matches the first m_{s_k} shifted moments around s_k and the first $\tilde{m}_{\tilde{s}_k}$ shifted moments around $\tilde{s}_k$ respectively

assuming the matrices $(s_k I_n - A)$ and $(\tilde{s}_k I_n - A)$ are invertible.

The proof of Theorem 1 can be found in [17]. A rational Lanczos process is given in algorithm 2. For simplicity we assume that $m_{s_k} = m_{\tilde{s}_k}$ and also it is assumed that $s_i \neq s_j$ and $\tilde{s}_i \neq \tilde{s}_j$ for $i \neq j$. As mentioned in section I, a drawback of rational methods is that no Lanczos-like equations exist. This issue has been investigated in [14], [15], [17], [18], where they give equations that describe the rational algorithms; however these equations are not in the standard Lanczos form. The work of this paper studies the same problems but it is based on the development of Lanczos-like equations for the rational case in the standard form. Residual error expressions can then be readily derived as in the case of standard Lanczos methods and adaptive algorithms are developed.

Algorithm 2 Rational Lanczos algorithm

Inputs: $S = \{s_1, \ldots, s_K\}$, $\tilde{S} = \{\tilde{s}_1, \ldots, \tilde{s}_K\}$
  $A, B, C, \epsilon, \quad m_{s_k} = m_{\tilde{s}_k}$
Initialize: $V_m = [\,]$, $W_m = [\,]$, $i = 0$
for $k = 1$ *to* K
  if $\{s_k = \infty\}$, $\hat{v}_{i+1} = B$
  else
    $\hat{v}_{i+1} = (s_k I_n - A)^{-1} B$
  end
  if $\{\tilde{s}_k = \infty\}$, $\hat{w}_{i+1} = C'$
  else
    $\hat{w}_{i+1} = ((\tilde{s}_k I_n - A)^{-1})' C'$
  end
  If $\{\sqrt{|\hat{w}_i'\hat{v}_i|} < \epsilon\}$, Stop **End**
  $v_{i+1} = \frac{\hat{v}_{i+1}}{\sqrt{|\hat{w}_{i+1}'\hat{v}_{i+1}|}}$, $w_{i+1} = \hat{w}_{i+1} / \frac{\hat{w}_{i+1}'\hat{v}_{i+1}}{\sqrt{|\hat{w}_{i+1}'\hat{v}_{i+1}|}}$
  $V_m = [V_m \;\; v_{i+1}], \qquad W_m = [W_m \;\; w_{i+1}]$
  $i = i + 1$
  for $j = 1$ *to* $m_{s_k} - 1$
    if $\{s_k = \infty\}$, $\hat{v}_{i+1} = A v_i$
    else
      $\hat{v}_{i+1} = (s_k I_n - A)^{-1} v_i$
    end
    if $\{\tilde{s}_k = \infty\}$, $\hat{w}_{i+1} = A' w_i$
    else
      $\hat{w}_{i+1} = ((\tilde{s}_k I_n - A)^{-1})' w_i$
    end
    $\hat{v}_{i+1} = \hat{v}_{i+1} - V_m W_m{}' \hat{v}_{i+1}$
    $\hat{w}_{i+1} = \hat{w}_{i+1} - W_m V_m{}' \hat{w}_{i+1}$
    $\rho = \sqrt{|\hat{w}_{i+1}'\hat{v}_{i+1}|}$
    If $\{\rho < \epsilon\}$, Stop **End**
    $\lambda = \frac{\hat{w}_{i+1}'\hat{v}_{i+1}}{\rho}$
    $v_{i+1} = \hat{v}_{i+1}/\rho, \qquad w_{i+1} = \hat{w}_{i+1}/\lambda'$
    $V_m = [\, V_m \;\; v_{i+1} \,]$, $W_m = [\, W_m \;\; w_{i+1} \,]$
    $i = i + 1$
  end
end
Outputs : $V_m = \{v_1, \ldots, v_m\}$,$W_m = \{w_1, \ldots, w_m\}$

III. LANCZOS AND ARNOLDI-LIKE EQUATIONS FOR RATIONAL INTERPOLATION

Rational interpolation generally provides a more accurate reduced-order model than interpolation around a single point since it is based on the combination of approximations around many interpolation points. The reduced-order model created by rational interpolation can be improved by a proper selection of these points. For this it is necessary to obtain frequency dependent error expressions. The interpolation points could then be the frequencies at which the error expressions are maximum using the $\mathcal{H}_\infty$ norm as measure. The aim is to create rapidly and efficiently accurate reduced order models. In [20] for example they develop an exact expression for the $\mathcal{H}_2$ norm of the error term. They suggest that by interpolating at the negative of the eigenvalues of A with the highest residues of the transfer function $G(s)$ the $\mathcal{H}_2$ is minimized. This method however requires the computation of the eigenvalues of the A matrix of the system which can be very slow when A is very large.

Many of the results based on Krylov subspaces follow from the Arnoldi and Lanczos equations of the standard Arnoldi and Lanczos algorithm. No results for extending these equations to the rational Arnoldi or Lanczos case exist in the literature. A main contribution of this work is to derive corresponding equations for the rational version of these algorithms. In this section we derive with minimum additional effort Arnoldi and Lanczos-like equations in the familiar form of the standard Arnoldi and Lanczos equations. The standard version of these equations allow us to have simple residual error expressions for the rational case.

A. Derivation of Lanczos equations in the rational case

The following Lemma derives a set of equations in the standard form for the Lanczos process for the rational case. Using these equations, the Lemma also provides expressions for the residuals errors. These expressions will prove crucial in deriving an adaptive rational Lanczos algorithm for choosing the frequencies at which the reduced order system matches the dynamics of the original system such that the approximation error tends to be reduced.

Lemma 1: Let V_m and W_m be as defined in Theorem 1 and let m_∞ and $\tilde{m}_\infty$ be the multiplicities of ∞ in $\mathcal{S}$ and $\tilde{\mathcal{S}}$, respectively. If we compute $V_{m+1} = [V_m \; v_{m+1}]$ and $W_{m+1} = [W_m \; w_{m+1}]$ such that

$$[V_m \mid A^{m_\infty} B] \subseteq \text{span}\{V_{m+1}\},$$
$$[W_m \mid (A^{\tilde{m}_\infty})' C'] \subseteq \text{span}\{W_{m+1}\},$$
$$W'_{m+1} V_{m+1} = I_{m+1},$$

then

$$AV_m = V_m A_m + v_{m+1} C_{V_m}, \tag{8}$$
$$B = V_m B_m + v_{m+1} b_m, \tag{9}$$
$$A' W_m = W_m A'_m + w_{m+1} B'_{W_m}, \tag{10}$$
$$C = C_m W'_m + c_m w'_{m+1}, \tag{11}$$

where $b_m = w'_{m+1} B$, $c_m = C v_{m+1}$, $C_{V_m} = w'_{m+1} A V_m$ and $B_{W_m} = W'_m A v_{m+1}$. Furthermore, $b_m = 0$ if $m_\infty > 0$ and $c_m = 0$ if $\tilde{m}_\infty > 0$.

Proof: We first prove the result for $m_\infty = 0$. Let V_m be defined as in Theorem 1. Then we extend V_m to $V_{m+1} = [V_m \mid v_{m+1}]$ such that

$$[V_m \mid B] \subseteq \text{span}\{V_{m+1}\}$$

by biorthogonalising B against all previous columns of W_m with the Lanczos algorithm. Then the following are true:

$$(s_1 I_n - A)^{-1} B \in \text{span}\{V_1\} \tag{12}$$
$$\vdots$$
$$(s_k I_n - A)^{-(i-1)} B \in \text{span}\{V_{j-1}\}$$
$$(s_k I_n - A)^{-i} B \in \text{span}\{V_j\} \tag{13}$$
$$\vdots$$
$$B \in \text{span}\{V_{m+1}\} \tag{14}$$

We start by proving the Lemma for the first column of V_m. Multiply (12) by $(s_1 I_n - A)$ from the left and rearrange to get

$$Av_1 \in \text{span}\{V_1, B\} \overset{(14)}{\Rightarrow} AV_1 \in \text{span}\{V_{m+1}\}.$$

We proceed the proof by induction. We assume that the result holds for an arbitrary interpolation point s_k of the $\mathcal{K}_{s_k}$ krylov subspace up to the $(i-1)_{th}$ multiplicity. We will prove the result for the next multiplicity and hence the proof will be complete. Therefore we assume

$$AV_{j-1} = A\,[v_1 \quad \ldots \quad v_{j-1}] \in \text{span}\{V_{m+1}\} \tag{15}$$

and then we prove that it is true for the next index j. Multiply (13) from the left by $(s_k I_n - A)$ and rearrange to get:

$$Av_j \in \text{span}\{V_j, AV_{j-1}\} \overset{(15)}{\Rightarrow} Av_j \in \text{span}\{V_{m+1}\}.$$

Combining the above with the assumption made in (15)

$$\Rightarrow AV_j \in \text{span}\{V_{m+1}\}. \tag{16}$$

Therefore it is easy to see that the result in (16) holds for all columns in V_m, i.e.,

$$AV_m \in \text{span}\{V_{m+1}\}. \tag{17}$$

To prove (8) we proceed as follows: Since $AV_m \in \text{span}\{V_{m+1}\}$ there exists a matrix $Y \in \mathcal{C}^{(m+1)\times m}$ such that

$$AV_m = V_{m+1} Y. \tag{18}$$

Partitioning Y as $\begin{bmatrix} A_m \\ C_{V_m} \end{bmatrix}$ and multiplying (18) by W'_{m+1} from the left, due to biorthogonality between W_{m+1} and V_{m+1} we get that $A_m = W'_m A V_m$ and $C_{V_m} = w'_{m+1} A V_m$

$$\Rightarrow AV_m = V_m A_m + v_{m+1} C_{V_m}.$$

Similarly to prove (9) we proceed as follows: Since $B \in \text{span}\{V_{m+1}\}$ there exists a matrix $Z \in \mathcal{C}^{(m+1)\times 1}$ such that

$$B = V_{m+1} Z. \tag{19}$$

Partitioning Z as $\begin{bmatrix} B_m \\ b_m \end{bmatrix}$ and multiplying (19) by W'_{m+1} from the left we have that $B_m = W'_m B$ and $b_m = w'_{m+1} B$.

$$\Rightarrow B = V_m B_m + v_{m+1} b_m$$

Therefore we have the first step of the proof for (8) and (9).

Next we prove the result for $m_\infty > 0$. Let the basis V_m be such that

$$[B\ AB\ \cdots\ A^{p-1}B\ \ V_{m-p}] \in \text{span}\{V_m\}$$

where V_{m-p} is as defined in Theorem 1. Since B is already in the span of V_m it is easy to see that (8) would hold if

$$\{Av_1, \ldots, Av_p\} \in \text{span}\{V_{m+1}\}. \tag{20}$$

This can be shown by extending V_m to $V_{m+1} = [V_m \mid v_{m+1}]$ such that

$$[V_m \mid A^p B] \in \text{span}\{V_{m+1}\} \quad \text{and} \quad W'_{m+1}V_{m+1} = I_{m+1}$$

by biorthogonalising A^pB against all the previous columns of W_m with the Lanczos algorithm. It follows that (20) holds since by construction we have that,

$$A^k B \in \begin{cases} \text{span}\{v_1, \ldots, v_{k+1}\}, & for\ 0 < k < p-1 \\ \text{span}\{v_1, \ldots, v_{m+1}\}, & for\ k = p-1 \end{cases}$$

which completes the proof of (8) and (9). To prove the last part, note that if $m_\infty > 0$ then $B \in \text{span}\{V_m\}$ from which it follows that $b_m = 0$.

The proof of Equations (10) and (11) is similar and it is therefore omitted. ■

B. Simplified Lanczos residual errors

With the use of Lemma 1, the residual errors $R_B(s)$ and $R_C(s)$ in (6) and (7) can now be simplified for the rational Lanczos procedure as

$$R_B(s) = v_{m+1}\{C_{V_m}(sI_m - A_m)^{-1}B_m + b_m\} \tag{21}$$
$$R_C(s) = w_{m+1}\{B'_{W_m}((sI_m - A_m)^{-1})'C'_m + c'_m\} \tag{22}$$

The residual errors in this case can be computed less expensively than the approximation errors, since only quantities related to the m_{th} order model are involved, compared to the approximation errors in the initial form which involve quantities related to an n_{th} order system. Also it is important to mention that Lemma 1 does not alter V_m or W_m and the only additional cost is an extra iteration of the Lanczos algorithm.

Using (8),(9), (10) and (11) we can derive the residual errors in (21) and (22) respectively.

$$\begin{aligned} R_B(s) &= B - (sI_n - A)V_m X_m(s) \\ &\overset{(8)}{=} B - V_m(sI_m - A_m)X_m(s) + v_{m+1}C_{V_m}X_m(s) \\ &\overset{(5),(9)}{=} v_{m+1}\{C_{V_m}(sI_m - A_m)^{-1}B_m + b_m\}. \end{aligned}$$

The derivation for $R_C(s)$ is similar and is omitted.

C. The Arnoldi-like equations

Following similar steps as for the derivation for the rational Lanczos case, we have developed Arnoldi-like equations for the rational Arnoldi case which are stated without proof in the following Lemma.

Lemma 2: Let V_m and W_m be as defined in Theorem 1 and let m_∞ and $\tilde{m}_\infty$ be the multiplicities of ∞ in $\mathcal{S}$ and $\tilde{\mathcal{S}}$, respectively. If we compute the orthogonal bases $V_{m+1} = [V_m\ v_{m+1}]$ and $W_{m+1} = [W_m\ w_{m+1}]$ such that

$$\begin{aligned} [V_m \mid A^{m_\infty}B] &\in \text{span}\{V_{m+1}\}, \\ V'_{m+1}V_{m+1} &= I_{m+1}, \\ [W_m \mid (A^{\tilde{m}_\infty})'C'] &\in \text{span}\{W_{m+1}\}, \\ W'_{m+1}W_{m+1} &= I_{m+1}, \end{aligned}$$

then

$$\begin{aligned} AV_m &= V_m E_m^{-1} A_m + (v_{m+1} - V_m E_m^{-1} W'_m v_{m+1}) C_{V_m}, \\ B &= V_m E_m^{-1} B_m + (v_{m+1} - V_m E_m^{-1} W'_m v_{m+1}) b_m, \\ W'_m A &= A_m E_m^{-1} W'_m + B_{W_m}(w'_{m+1} - w'_{m+1} V_m E_m^{-1} W'_m), \\ C &= C_m E_m^{-1} W'_m + c_m(w'_{m+1} - w'_{m+1} V_m E_m^{-1} W'_m) \end{aligned}$$

where $E_m = W'_m V_m$, $b_m = v'_{m+1}B$, $c_m = Cw_{m+1}$, $C_{V_m} = v'_{m+1}AV_m$, and $B_{W_m} = W'_m A w_{m+1}$.

D. Simplified Arnoldi residual errors

The residual errors $R_B(s)$ and $R_C(s)$ in this case can be simplified as

$$\begin{aligned} R_B(s) &= (v_{m+1} - V_m E_m^{-1} W'_m v_{m+1}) \times \\ &\qquad \{C_{V_m}(sE_m - A_m)^{-1}B_m + b_m\} \\ R_C(s) &= (w_{m+1} - W_m (E_m^{-1})' V'_m w_{m+1}) \times \\ &\qquad \{B'_{W_m}((sE_m - A_m)^{-1})'C'_m + c'_m\}. \end{aligned}$$

IV. Adaptive Krylov algorithms for model reduction

The problem in adaptive rational methods is to decide on the next interpolation point on every iteration. In this section a number of options are described for the selection of the interpolation points. The choice may depend on the computational power or time restrictions required. The proposed methods are based in the idea that the interpolation points should be selected such that the approximation error mentioned in Section I in equation (4) should be minimized at every iteration in terms of a suitable norm. The error expression in (4) is rewritten below for convenience

$$\epsilon(s) = R_C(s)'(sI_n - A)^{-1}R_B(s).$$

In Section III simple expression terms for the residual errors were derived, involving quantities related to the reduced order model only. Let $\tilde{R}_C$ and $\tilde{R}_B$ be the frequency dependent terms of the residual errors and $\tilde{B}$ and $\tilde{C}$ the non-frequency dependent terms of the residual errors. In the Arnoldi case

$$\begin{aligned} \tilde{R}_B(s) &= C_{V_m}(sE_m - A_m)^{-1}B_m + b_m \\ &\overset{s}{=} \left[\begin{array}{cc|c} E_m & A_m & B_m \\ \hline * & C_{V_m} & b_m \end{array}\right], \\ \tilde{R}'_C(s) &= C_m(sE_m - A_m)^{-1}B_{W_m} + c_m \\ &\overset{s}{=} \left[\begin{array}{cc|c} E_m & A_m & B_{W_m} \\ \hline * & C_m & c_m \end{array}\right] \\ \tilde{B} &= v_{m+1} - V_m E_m^{-1} W'_m v_{m+1}, \\ \tilde{C} &= w'_{m+1} - w'_{m+1} V_m E_m^{-1} W'_m \end{aligned}$$

whereas in the Lanczos case

$$\begin{aligned}\tilde{R}_B(s) &= C_{V_m}(sI_m - A_m)^{-1}B_m + b_m \\ &\overset{s}{=} \left[\begin{array}{c|c} A_m & B_m \\ \hline C_{V_m} & b_m \end{array}\right] \\ \tilde{R}'_C(s) &= C_m(sI_m - A_m)^{-1}B_{W_m} + c_m \\ &\overset{s}{=} \left[\begin{array}{c|c} A_m & B_{W_m} \\ \hline C_m & c_m \end{array}\right], \\ \tilde{B} &= v_{m+1}, \\ \tilde{C} &= w'_{m+1},\end{aligned}$$

where C_{V_m}, B_{W_m}, b_m and c_m for each of the two methods are as defined in Lemmas 1 and 2.

Now the error expression in (4) becomes

$$\begin{aligned}\epsilon(s) &= \tilde{R}'_C(s)\tilde{C}(sI_n - A)^{-1}\tilde{B}\tilde{R}_B(s) \\ &= \tilde{R}'_C(s)H(s)\tilde{R}_B(s)\end{aligned}$$

where

$$H(s) \overset{s}{=} \left[\begin{array}{c|c} A & \tilde{B} \\ \hline \tilde{C} & 0 \end{array}\right].$$

As already mentioned the idea is to select an interpolation point at every iteration such that $\epsilon(s)$ is small in some norm. Ideally we would like, at every iteration, to find the frequency at which $\epsilon(s)$ achieve its maximum and then use this frequency as the next interpolation frequency for the Krylov methods. $\tilde{R}_C(s)$ and $\tilde{R}_B(s)$ are small terms involving quantities related to the reduced order model, but $H(s)$ contains terms related to the original system. Thus a computation of $\|\tilde{R}'_C H \tilde{R}_B\|_\infty$ on every iteration for medium and large scale systems is computationally very expensive. Therefore instead of using $H(s)$ we suggest using its approximation $\hat{H}(s)$.

The approximation of the error $\epsilon(s)$ does not necessarily have to be $\hat{\epsilon}(s) = \tilde{R}'_C(s)\hat{H}(s)\tilde{R}_B(s)$. The error approximation $\hat{\epsilon}(s)$ can be one of the expressions listed in Table I.

TABLE I
ERROR EXPRESSIONS

1	$\hat{\epsilon}(s) = \tilde{R}_B(s)$
2	$\hat{\epsilon}(s) = \tilde{R}_C(s)'$
3	$\hat{\epsilon}(s) = \hat{H}(s)\tilde{R}_B(s)$
4	$\hat{\epsilon}(s) = \hat{H}(s)$
5	$\hat{\epsilon}(s) = \tilde{R}_C(s)'\hat{H}(s)$
6	$\hat{\epsilon}(s) = \tilde{R}_C(s)'\hat{H}(s)\tilde{R}_B(s)$

In all cases the interpolation points are selected to be the frequencies $s \in \mathcal{C}$ and $\tilde{s} \in \mathcal{C}$ at which one of the approximated error expressions achieve its maximum, i.e.,

$$\mathcal{S} = \{s : |\hat{\epsilon}(s)| = \|\hat{\epsilon}\|_\infty\} \text{ and } \tilde{\mathcal{S}} = \{s : |\hat{\epsilon}(s)| = \|\hat{\epsilon}\|_\infty\}$$

where $\mathcal{S}$ and $\tilde{\mathcal{S}}$ denote the set of interpolation points as defined in Theorem 1. In the case where we are interested in a range of frequencies, then the interpolated points can be selected to be the frequencies at which a weighed approximated error $\hat{\epsilon}_W(s) = W_o\hat{\epsilon}(s)W_i$ achieve its maximum, where W_o, W_i are stable filters.

We suggest approximating $H(s)$ using the projection $P = \tilde{V}(\tilde{W}'\tilde{V})^{-1}\tilde{W}'$ with the Arnoldi or Lanczos algorithms as

$$\hat{H}(s) = \tilde{C}\tilde{V}(s\tilde{W}'\tilde{V} - \tilde{W}'A\tilde{V})^{-1}\tilde{W}'\tilde{B}$$

so that it includes small terms only. Note that in the Lanczos case $\tilde{W}'\tilde{V} = I$. The projection method to approximate $H(s)$ depends on the computational power and the time constrains. Below there is a list of different suggestions for approximating $\hat{H}(s)$.

- On every iteration approximate $H(s)$ by standard rational Arnoldi or Lanczos algorithms using the set of frequencies $\mathcal{S}$ and $\tilde{S}$ already computed so far. As the algorithm progresses the approximation of $H(s)$ is improved.
- Instead of computing $\hat{H}(s)$ by applying rational interpolation on $H(s)$ on every iteration which requires long computional time we can perform Arnoldi or Lanczos algorithm to match only at the last frequencies added in $\mathcal{S}$ and $\tilde{\mathcal{S}}$. Therefore in this case:

  $$\tilde{V} = \tilde{v}, \quad \text{and} \quad \tilde{W} = \tilde{w}.$$

- $\hat{H}(s)$ can also be projected with $\tilde{V}$ and $\tilde{W}$ as:

  $$\tilde{V} = [V_m \mid \tilde{v}], \quad \text{and} \quad \tilde{W} = [W_m \mid \tilde{w}].$$

  where $\tilde{v}$ and $\tilde{w}$ are obtained as described in the previous method.
- As an alternative we suggest to approximate $H(s)$ by using the already computed columns w_{m+1} and v_{m+1}:

  $$\tilde{V} = v_{m+1}, \quad \text{and} \quad \tilde{W} = w_{m+1}$$

- Finally we also suggest that $\hat{H}(s)$ can be projected with $\tilde{V}$ and $\tilde{W}$ as the already computed bases W_{m+1} and V_{m+1}:

  $$\tilde{V} = V_{m+1}, \quad \text{and} \quad \tilde{W} = W_{m+1}.$$

A pseudocode for the algorithm for the adaptive rational method, is given in algorithm 3.

A. *Numerical Examples*

Figure 1 shows the magnitude of the bode plot of a randomly generated system of order $n = 150$, the magnitude plot of the reduced order system using the standard rational Arnoldi method as well as the magnitude of the error. In this example it was assumed that there was no previous knowledge on the characteristics of the transfer function of the original system. Therefore the standard Arnoldi rational algorithm was applied to match 4 moments at ten equally spaced (on logarithmic scale) interpolation points $\mathcal{S} = \tilde{\mathcal{S}} = \{10^{-4}j, 10^{-3}j, \ldots, 10^5 j\}$. It can be seen that the approximation is not satisfactory. Figure 2 shows the bode plot of the original system, of the reduced order system using the adaptive algorithm developed in this paper and of

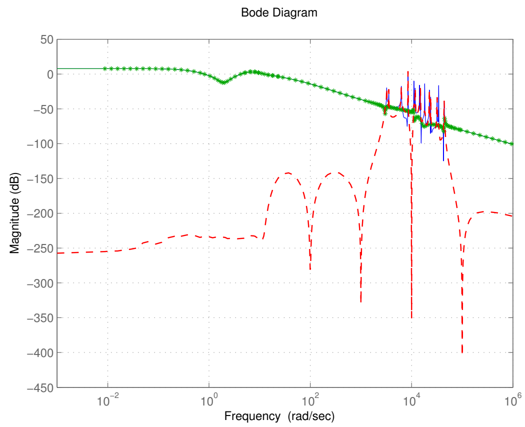

Fig. 1. Bode Diagram of the transfer functions of the actual system (continuous line), of the reduced order system obtained by standard rational Krylov method (dotted line), and of the error between them (dashed line). The order of the original system is $n = 150$ and of reduced order system is $m = 40$.

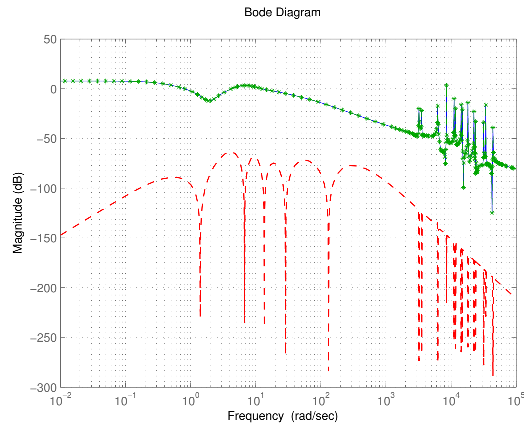

Fig. 2. Bode Diagram of the transfer functions of the actual system (continuous line), of the reduced order system obtained by the adaptive rational Krylov method (dotted line), and of the error between them (dashed line). The order of the original system is $n = 150$ and of reduced order system is $m = 40$.

the error. It can be clearly seen that the adaptive algorithm has a better performance.

It is important to note that in practice there is usually no previous knowledge of the original system frequency response. Applying model approximation using the adaptive algorithm presented in this paper results in reduced models with little redundant information and improves the overall performance of the Krylov reduction methods. It is essential that the extra cost of the adaptive algorithm is small due to speed and storage limitations. In this paper we have developed an adaptive method for a fast computation of the next interpolation frequency using the simple error expressions developed in this paper.

Table II gives a comparison of the approximation error $\|G(s) - G_m(s)\|_\infty$ of the methods described in this paper. In all cases the algorithms were performed in real arithmetic [13] and a stable projection was applied to the reduced system. Note that if $\tilde{V} \in \mathcal{C}^{n\times m}$ is a base of a subspase then $V = [real\{\tilde{V}\} \quad imag\{\tilde{V}\}] \in \mathcal{R}^{n\times 2m}$ is also a base of the same subspace. Therefore in this part a complex basis is converted to a real one before projecting the original system. As can be seen from the results in Table II, in all the cases where the error involves $\hat{H}(s)$ and a residual error the approximation error is comparable or better than the error obtained by balanced truncation. Our numerical experience indicates that this tends to be the case when the size of V_m and W_m is large enough to give a good approximation, otherwise for very low m balance truncation gives better results.

Algorithm 3 Adaptive rational method pseudo-code

1: Inputs : A, B, C, m
2: Choose initial frequencies to match, e.g. $s_1 = \infty$ and $\tilde{s}_1 = \infty$
3: **for** i=1 to m
4: Compute v_m and w_m by rational Lanczos (or Arnoldi) method to match at s_i and $\tilde{s}_i$.
5: Generate the Lanczos (or Arnoldi) equations as described by Lemma 1 (or 2).
6: Use one of the error expressions in Table I to compute next interpolation frequencies s_{i+1} and $\tilde{s}_{i+1}$
7: If the infinity norm of the error expression used is below a threshold **stop**.
8: **end**
9: Outputs : $A_m = W_m{}'AV_m$, $E_m = W_m{}'V_m$, $B_m = W_m{}'B$ and $C_m = CV_m$

V. CONCLUSIONS

The work of this paper derives Arnoldi and Lanczos-like equations for the rational versions of these algorithms. Simple residual error expressions have also been developed which are used for computing the interpolation frequencies at which the moments of the original system are to be matched. The simple error expressions derived in this paper contain only terms of the reduced order system and this allows fast computations. This selection of the interpolation points reduces the overall approximation error compared to standard rational methods and conventional methods; the adaptive method developed tends to reduce the error in the range of frequencies of interest without a priori knowledge of the original system frequency response.

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TABLE II

COMPARISON, $n = 250$, $m = 50$

Error Expressions using Residual Error information only	$\|G - G_m\|_\infty$
$\mathcal{S} = \{s\ :\ \|\tilde{R}_B(s)\| = \|\tilde{R}_B\|_\infty\}$, $\tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}_C(s)\| = \|\tilde{R}_C\|_\infty\}$	4.8196×10^{-09}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}_B(s)\| = \|\tilde{R}_B\|_\infty\}$	3.9485×10^{-09}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}_C(s)\| = \|\tilde{R}_C\|_\infty\}$	1.1583×10^{-08}
Error Expressions using $\hat{H}(s)$ projected with $\tilde{V} = v_{m+1}$ and $\tilde{W} = w_{m+1}$	
$\{\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\| = \|\hat{H}\|_\infty\}$	0.8713
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\tilde{R}_B(s)\| = \|\hat{H}\tilde{R}_B\|_\infty\}$	5.7186×10^{-09}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}'_C(s)\hat{H}(s)\| = \|\tilde{R}'_C\hat{H}\|_\infty\}$	1.2372×10^{-05}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{\epsilon}(s)\| = \|\tilde{R}'_C\hat{H}\tilde{R}_B\|_\infty\}$	3.5906×10^{-07}
Error Expressions using $\hat{H}(s)$ projected with $\tilde{V} = V_{m+1}$ and $\tilde{W} = W_{m+1}$	
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\| = \|\hat{H}\|_\infty\}$	1.4916×10^{-05}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\tilde{R}_B(s)\| = \|\hat{H}\tilde{R}_B\|_\infty\}$	1.4660×10^{-07}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}'_C(s)\hat{H}(s)\| = \|\tilde{R}'_C\hat{H}\|_\infty\}$	9.5817×10^{-07}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{\epsilon}(s)\| = \|\tilde{R}'_C\hat{H}\tilde{R}_B\|_\infty\}$	2.9304×10^{-07}
Error Expressions using $\hat{H}(s)$ projected with $\tilde{V} = [\tilde{v}]$ and $\tilde{W} = [\tilde{w}]$	
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\| = \|\hat{H}\|_\infty\}$	5.7132×10^{-07}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\tilde{R}_B(s)\| = \|\hat{H}\tilde{R}_B\|_\infty\}$	1.6118×10^{-07}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}'_C(s)\hat{H}(s)\| = \|\tilde{R}'_C\hat{H}\|_\infty\}$	5.5497×10^{-08}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{\epsilon}(s)\| = \|\tilde{R}'_C\hat{H}\tilde{R}_B\|_\infty\}$	2.0735×10^{-07}
Error Expressions using $\hat{H}(s)$ projected with $\tilde{V} = [V_m\ \|\ \tilde{v}]$ and $\tilde{W} = [W_m\ \|\ \tilde{w}]$	
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\| = \|\hat{H}\|_\infty\}$	0.8713
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\tilde{R}_B(s)\| = \|\hat{H}\tilde{R}_B\|_\infty\}$	6.4628×10^{-09}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}'_C(s)\hat{H}(s)\| = \|\tilde{R}'_C\hat{H}\|_\infty\}$	5.7443×10^{-09}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{\epsilon}(s)\| = \|\tilde{R}'_C\hat{H}\tilde{R}_B\|_\infty\}$	2.8055×10^{-07}
Error Expressions using $\hat{H}(s)$ projected with $\tilde{V}$ and $\tilde{W}$ computed by rational interpolation	
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\| = \|\hat{H}\|_\infty\}$	0.6258
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{H}(s)\tilde{R}_B(s)\| = \|\hat{H}\tilde{R}_B\|_\infty\}$	8.0936×10^{-06}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\tilde{R}'_C(s)\hat{H}(s)\| = \|\tilde{R}'_C\hat{H}\|_\infty\}$	4.4379×10^{-07}
$\mathcal{S} = \tilde{\mathcal{S}} = \{s\ :\ \|\hat{\epsilon}(s)\| = \|\tilde{R}'_C\hat{H}\tilde{R}_B\|_\infty\}$	2.5666×10^{-08}
Balanced Truncation	8.8916×10^{-06}
Rational Krylov : interpolation points $S = \tilde{S} = \{10^{-4}j, \ldots, 10^{5}j\}$, $multiplicity = 5$	0.8714

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