Some Remarks on A Priori Error Estimation for ESVDMOR

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Abstract In previous work it is shown how to numerically improve the ESVDMOR method of Feldmann and Liu to be really applicable to linear, sparse, very large scale, and continuous-time descriptor systems. Stability and passivity preservation of this algorithm is also already proven. This work presents some steps towards a global a priori error estimation for this algorithm, which is necessary for a fully automatic application of this approach.

1 Motivation

Although model order reduction (MOR) for linear time invariant (LTI) systems is a well investigated area of research [1], most of the established approaches, e.g., Krylov subspace methods or balanced truncation methods [7], are not able to work on systems with a lot of input and output terminals. They are not easily reducible, especially really large scale ones. ESVDMOR is, besides other approaches [5], a MOR approach to reduce linear systems with a large number of terminals [2–4, 6]. Within the algorithm, approximation errors are caused at different steps. The magnitude of these errors can be influenced with the help of different decisions. Some of the correlations between these decisions and the influence on the results are well known, but a closed error analysis for the ESVDMOR approach does

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not yet exist. For efficient reduction which meets the requirements placed on the reduced order model, the knowledge about this correlations is of essential relevance. The goal is to get a reduced model which is as small as possible and at the same time as good as necessary. This knowledge is essential for the industrial usage of MOR algorithms. In Sect. 2 we briefly repeat required basic knowledge including the steps of SVDMOR and ESVDMOR. We emphasize those steps which cause an approximation error in some way. The following section deals with the single errors and the known theory. We combine all influences, firstly with a lot of assumptions and for the easy cases and later for more complicated models, to get ideas about a global error bound for the ESVDMOR approach.

2 (E)SVDMOR Basics Including Error Sources

Starting point is a given (mostly by modeling in circuit simulation but also in mechanical, biological, and chemical applications) linear time-invariant continuous-time descriptor system

$$\begin{aligned} C\dot{x}(t) &= -Gx(t) + Bu(t),\ x(0) = x_0, \\ y(t) &= Lx(t), \end{aligned} \tag{1}$$

where $C, G \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m_{in}}$, $L \in \mathbb{R}^{m_{out}\times n}$. Vector $x(t) \in \mathbb{R}^n$ contains the descriptor variables, $u(t) \in \mathbb{R}^{m_{in}}$ is the vector of inputs, $y(t) \in \mathbb{R}^{m_{out}}$ is the output vector, and $x_0 \in \mathbb{R}^n$ is the initial value. The value n is called order of (1) defined by the number of descriptor variables and m_{in} and m_{out} denote the number of I/O terminals, respectively. System (1) has the following transfer function in frequency domain:

$$H(s) = L(sC + G)^{-1}B, \tag{2}$$

which we get from (1) for $x_0 = 0$ by applying the Laplace transform. Like mentioned in Sect. 1 we want to investigate systems with

$$m_{in/out} \sim n.$$

Further on, we define the *i-th block moment of (2)* as $\mathbf{m_i} = L(-G^{-1}C)^i G^{-1}B$, $i = 0, 1, \ldots$, in terms of $\mathbf{m_i}$ as an $m_{out} \times m_{in}$ matrix. These moments are equal to the coefficients of the Taylor series expansion of (2) about $s_0 = 0$, $H(s) = \sum_{i=0}^{\infty} m_i s^i$. For $s_0 \neq 0$ this leads to *frequency shifted moments* defined as

$$\mathbf{m_i}(s_0) = L(-(s_0C + G)^{-1}C)^i (s_0C + G)^{-1}B, \qquad i = 0, 1, \ldots$$

Thus, the Taylor series expansion including these moments is

$$H(s) = \sum_{i=0}^{\infty} m_i (s - s_0)^i .$$

To allow terminal reduction for inputs and outputs separately, w.l.o.g. we use r different (frequency shifted) block moments forming two moment or ansatz matrices, the input response matrix M_I and the output response matrix M_O, as follows:

$$M_I = \begin{bmatrix} \mathbf{m_0} \\ \mathbf{m_1} \\ \vdots \\ \mathbf{m_{r-1}} \end{bmatrix}, \qquad M_O = \begin{bmatrix} \mathbf{m_0}^T \\ \mathbf{m_1}^T \\ \vdots \\ \mathbf{m_{r-1}}^T \end{bmatrix}. \tag{3}$$

It is also possible to use different numbers of block moments to create M_I and M_O. The number r is the first possibility to influence the accuracy of the reduced model. For simplicity, we assume the number of rows in M_I and M_O of (3) to be larger than the number of columns, i.e., $r \cdot m_{out} \geq m_{in}$ and $r \cdot m_{in} \geq m_{out}$. If not, r has to be increased. Applying the SVD to these matrices, we obtain a low rank approximation

$$M_I \approx U_{I_{r_i}} \Sigma_{I_{r_i}} V_{I_{r_i}}^T \quad \text{and} \quad M_O \approx U_{O_{r_o}} \Sigma_{O_{r_o}} V_{O_{r_o}}^T, \tag{4}$$

which causes an approximation error. The matrices $\Sigma_{I_{r_i}}$ and $\Sigma_{O_{r_o}}$ are $r_i \times r_i$ and $r_o \times r_o$ diagonal matrices, $V_{I_{r_i}}$ and $V_{O_{r_o}}$ are $m_{in} \times r_i$ and $m_{out} \times r_o$ isometric matrices that contain the dominant column subspaces of M_I and M_O, and $U_{I_{r_i}}$ and $U_{O_{r_o}}$ are $r \cdot m_{out} \times r_i$ and $r \cdot m_{in} \times r_o$ isometric matrices that are not used any further. The values $r_i \leq m_{in}$ and $r_o \leq m_{out}$ denote the numbers of significant singular values (SV) as well as the numbers of the virtual input and output terminals of the terminal reduced order model. Due to the fact that the important information about the dependencies of the I/O-ports is hidden in the matrices $V_{I_{r_i}}^T$ and $V_{O_{r_o}}^T$, we use these matrices to find the searched approximate factorization of B and L. Hence, $B = BI \approx B(V_{I_{r_i}} V_{I_{r_i}}^+)$, where I denotes the identity matrix and $()^+$ denotes the Moore-Penrose pseudoinverse. Using the properties of this pseudoinverse and $(V_{I_{r_i}}^T V_{I_{r_i}})^{-1} = I$ leads to $B \approx B V_{I_{r_i}} (V_{I_{r_i}}^T V_{I_{r_i}})^{-1} V_{I_{r_i}}^T = B V_{I_{r_i}} V_{I_{r_i}}^T$. Defining a matrix B_r as $B_r := B V_{I_{r_i}}$ we finally get the approximation $B \approx B_r V_{I_{r_i}}^T$. Equivalent arguments lead to $L \approx V_{O_{r_o}} L_r$ with $L_r = V_{O_{r_o}}^T L$. The approximation errors which appear in these equations are very important, see Sect. 3. Plugging in these approximations in (2), we consequently get a new internal transfer function $H_r(s)$ by using the approximation

$$H(s) \approx \widehat{H}(s) = V_{O_{r_o}} \underbrace{L_r (G + sC)^{-1} B_r}_{:= H_r(s)} V_{I_{r_i}}^T .$$

This terminal reduced transfer function $H_r(s)$ can be further reduced to

$$\tilde{H}_r(s) = \tilde{L}_r(\tilde{G} + s\tilde{C})^{-1}\tilde{B}_r \approx H_r(s) \tag{5}$$

by any established MOR method. Balanced truncation approaches are advantageous as there exists a well known error theory, see Sect. 3. We end up with a very compact terminal reduced and reduced-order model $\tilde{H}_r(s)$, i. e.

$$H(s) \approx \widehat{H}(s) = V_{O_{r_o}} H_r(s) V_{I_{r_i}}^T \approx \widehat{H}_r(s) = V_{O_{r_o}} \tilde{H}_r(s) V_{I_{r_i}}^T. \tag{6}$$

3 Bounds for Particular Approximation Errors and Global ESVDMOR Error Bound

In this section we recall known facts about the errors mentioned in Sect. 2. We give ideas how to connect these errors to a global error bound for ESVDMOR. To get an appropriate entrance in the subject matter we recall two needed matrix norms.

Definition 1 (Spectral norm). The *spectral norm* of the transfer function (2) is induced by the Euclidean vector norm and defined as

$$||H(s)||_2 = \sqrt{\lambda_{\max}(H(s)^H H(s))},$$

where H^H denotes the conjugate transpose of H and $\lambda_{\max}$ denotes its largest eigenvalue.

Another very useful and important norm is based on the Hardy Space theory.

Definition 2 ($\mathscr{H}_\infty$-norm). Let $\mathbb{C}_+$ be the open right half plane. The $\mathscr{H}_\infty$*-norm* of the transfer function (2) is defined as

$$||H||_{\mathscr{H}_\infty} = \sup_{s\in\mathbb{C}_+} \sigma_{\max}(H(s)) = \sup_{s\in\mathbb{C}_+} ||H(s)||_2, \tag{7}$$

where σ_{max} denotes the largest singular value. Because of the maximum modulus theorem we can express (7) as $||H||_{\mathscr{H}_\infty} = \sup_{\omega\in\mathbb{R}} \sigma_{\max}(H(i\omega))$.

3.1 Particular Error Bounds

Equation (4) describes a truncated singular value decomposition (SVD). We know the error caused by a SVD of M_I is

$$e_{M_I} = \left\| M_I(r) - U_{I_{r_i}} \Sigma_{r_i}^I V_{I_{r_i}}^T \right\|_2 = \sigma_{r_i+1}^I,$$

where

$$\Sigma^I = \mathrm{diag}(\sigma_i^I) \approx \Sigma_{r_i}^I = \mathrm{diag}(\sigma_j^I),$$

with $i = 1, \dots, m_{in}$ and $j = 1, \dots, r_i$, and $\sigma_1^I \geq \dots \geq \sigma_{r_i}^I \geq \sigma_{r_{i+1}}^I \geq \dots \geq \sigma_{m_{in}}^I \geq 0$. The same applies to M_O. Here, the notation $M_I(r)$ expresses the dependency on the number r of used block moments m_i.

Another well known error can be found in (5) if we use a suitable method which gives the information, e. g., balanced truncation (BT) methods. The use of these methods leads to a reduction based on the truncation of the so called Hankel SVs. Provided that G is invertible, we get these values by balancing the controllability and the observability Gramian of H_r in the following form:

$$P = Q =: \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} = \mathrm{diag}(\hat{\sigma_1}, \dots, \hat{\sigma_n}).$$

Due to storage, efficiency and accuracy reasons usually one computes approximate low rank factors $P \approx P_C P_C^T$ and $Q \approx Q_C Q_C^T$. Using these factors, we compute a singular value decomposition of the form

$$Q_C^T C P_C = \begin{bmatrix} U_1 \; U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}.$$

Now we define the balancing transformations

$$T_l = Q_C U_1 \Sigma_1^{-1/2} \quad \text{and} \quad T_r = P_C V_1 \Sigma_1^{-1/2},$$

where $\Sigma_1^{-1/2} = \mathrm{diag}(\frac{1}{\sqrt{\hat{\sigma_1}}}, \dots, \frac{1}{\sqrt{\hat{\sigma_l}}})$, such that we are able to compute the reduced system as

$$(\tilde{C}, \tilde{G}, \tilde{B}_r, \tilde{L}_r) := (T_l^T C T_r, T_l^T G T_r, T_l^T B_r, L_r T_r).$$

The error for this square root variant of balanced truncation is bounded by

$$\left\| H_r - \tilde{H}_r \right\|_{\mathscr{H}_\infty} \leq 2 \sum_{k=l+1}^{n} \hat{\sigma_k} = \delta, \tag{8}$$

in case we keep the l largest $\hat{\sigma_i}$. A proof can be found, e.g., in [1]. Figure 1 shows a system with $n = 500$ states, $m_{in} = 5$ inputs, $m_{out} = 10$ outputs and it is reduced to order $l = 60$. The computed error bound is $\delta = 9.796 \cdot 10^{-3}$. The error does not even reach the bound.

3.2 Total Error Bound

Due to (6) and the triangle inequality the total ESVDMOR error in spectral norm on the imaginary axis can be expressed locally as

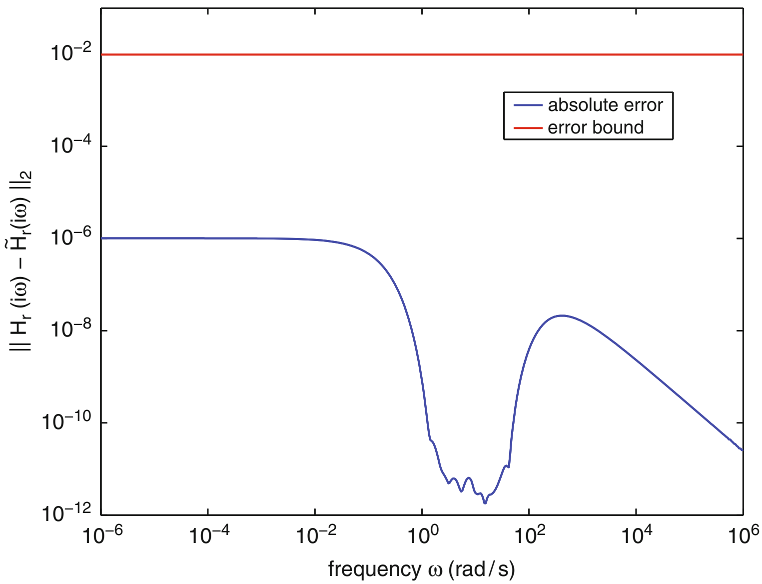

Fig. 1 Absolute error of a BT reduced system

$$e_{tot} = \left\| H(i\omega) - \hat{H}_r(i\omega) \right\|_2 \leq \underbrace{\left\| H(i\omega) - \hat{H}(i\omega) \right\|_2}_{=e_{out}} + \underbrace{\left\| \hat{H}(i\omega) - \hat{H}_r(i\omega) \right\|_2}_{e_{in}}. \tag{9}$$

The BT part (the error caused by the inner reduction e_{in}) follows from (6), (8), (9)

$$e_{in} = \left\| V_{O_{r_o}} H_r(s) V_{I_{r_i}}^T - V_{O_{r_o}} \tilde{H}_r(s) V_{I_{r_i}}^T \right\|_2 = \left\| H_r(s) - \tilde{H}_r(s) \right\|_2 \leq \delta,$$

due to the fact the spectral norm is invariant under orthogonal transformations. The terminal reduction part, also called outer reduction error e_{out}, turns out to be more complicated. To keep things simple we assume dealing with RLC circuits only, i. e., $m_{in} = m_{out} = m$, $L = B^T$, and, if $s_0 C + G \geq 0$, consequently $H(s) = H(s)^T$. Due to symmetry, $M_I = M_O = U\Sigma V^T$, and also $V_I = V_O = V$. Moreover $U = V$ holds in the SVDMOR case, which means that there is only one m_i in the ansatz matrices ($r = 1$), e.g. m_0 and $s = s_0 \in \mathbb{R}$ such that

$$M_I = M_O^T = m_0 = B^T(s_0 C + G)^{-1} B = U\Sigma V^T = U\Sigma U^T \approx U_r \Sigma_r U_r^T.$$

The local terminal reduction error e_{out} then is

$$e_{out} = \left\| H - \hat{H} \right\|_2 = \left\| B^T(s_0 C + G)^{-1} B - U_r B_r^T (s_0 C + G)^{-1} B_r V_r^T \right\|_2$$

$$
\begin{aligned}
&\overset{\text{(U=V)}}{=} \left\| B^T(s_0C+G)^{-1}B - U_rU_r^TB^T(s_0C+G)^{-1}BU_rU_r^T \right\|_2 \\
&= \left\| U\Sigma U^T - U_rU_r^TU\Sigma U^TU_rU_r^T \right\|_2 = \left\| U\Sigma U^T - U_r\Sigma_rU_r^T \right\|_2 \\
&\overset{\text{(SVD)}}{=} \sigma_{k+1}^{I/O},
\end{aligned}
$$

if we keep k singular values or terminals. The total error in the SVDMOR case in spectral norm then is

$$
e_{tot} \le \sigma_{k+1}^{I/O} + 2\sum_{j=l+1}^{n} \hat{\sigma}_j. \tag{10}
$$

In the ESVDMOR case we allow $r \ge 1$ (r times m_i within the ansatz matrices), for simplicity let us assume $r = 3$ and m_0, m_1, and m_2. Thus,

$$
\begin{aligned}
M_I = \begin{pmatrix} m_0 \\ m_1 \\ m_2 \end{pmatrix} = \begin{pmatrix} U^{(1)} \\ U^{(2)} \\ U^{(3)} \end{pmatrix} \Sigma V &= \begin{pmatrix} U_1^{(1)} & U_2^{(1)} \\ U_1^{(2)} & U_2^{(2)} \\ U_1^{(3)} & U_2^{(3)} \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} \\
&=: \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix},
\end{aligned}
$$

where the row partitioning in U is as in M_I, M_O and the column partitioning refers to the number of kept singular values, call this number k. We get $m_j = U^{(j)}\Sigma V^T$, $j = 1, 2, 3$, (which is not an SVD as $U^{(j)}$ is not orthogonal, but $\|U^{(j)}\|_2 \le 1$ holds.) Thus we can write

$$
\begin{aligned}
H(s) - \hat{H}(s) &= \sum_{j=0}^{\infty} (m_j - \hat{m}_j)(s-s_0)^j \\
&= (m_0 - \hat{m}_0) + (m_1 - \hat{m}_1)(s-s_0) + (m_2 - \hat{m}_2)(s-s_0)^2 + \mathcal{O}(s-s_0)^3.
\end{aligned}
$$

We are now able to bound the first expressions. We write $P_1 = V_1V_1^T$, hence $I - P_1 = V_2V_2^T$, thus,

$$
\begin{aligned}
m_j - \hat{m}_j &= m_j - P_1m_jP_1 = U^{(j)}\Sigma V^T - P_1U^{(j)}\Sigma V^TV_1V_1^T \\
&= U^{(j)} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} - P_1U^{(j)} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} I_k \\ 0 \end{pmatrix} V_1^T \\
&= U^{(j)} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} + U^{(j)} \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} - P_1U^{(j)} \underbrace{\begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} V_1^T}_{= \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}}
\end{aligned}
$$

$$= U^{(j)} \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_2 \end{pmatrix} V^T + (I - P_1) U^{(j)} \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} V_1^T$$

$$= U^{(j)} \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_2 \end{pmatrix} V^T + V_2 V_2^T U^{(j)} \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} V_1^T =: e_{j,1} + e_{j,2}.$$

We can now express the error as follows:

$$H(s) - \hat{H}(s) = e_{0,1} + e_{1,1}(s - s_0) + e_{2,1}(s - s_0)^2$$
$$+ e_{0,2} + e_{1,2}(s - s_0) + e_{2,2}(s - s_0)^2 + \mathcal{O}(s - s_o)^3,$$

where, when taking norms, and using $\|U^{(j)}\|_2 \leq 1$, $\|V^T\|_2 = 1$,

$$\|e_{j,1}\|_2 \leq \sigma_{k+1}.$$

Unfortunately, the terms $\|e_{j,2}\|_2$ can not be bounded in a meaningful way. But if σ_{k+1} were zero, then $V_2 V_2^T$ projects onto the nullspace of M_I, so that if σ_{k+1} is small enough, $V_2 V_2^T$ is still an orthoprojector onto the joint approximate nullspace of the first r moments. That is, the error, up to order $r - 1$, is essentially contained in the nullspace of the first r moments. Future investigations will focus on exploiting this fact to get a general a priori error bound.

4 Conclusions

In this rather theoretical work we explain and reveal all important matters to get an error bound for the ESVDMOR approach. Although, we are not able to find a universal total error bound in all cases, in (10) we find an expression for the total error in spectral norm. With the help of the results in [8], which states that for some linear RLC circuits $||H||_{\mathcal{H}_\infty} = ||H(0)||_2$, our results are interesting and provide a total a priori SVDMOR error bound in $\mathcal{H}_\infty$-norm, as

$$\left\| H - \widehat{H}_r \right\|_{\mathcal{H}_\infty} = \sup_{\omega \in \mathbb{R}} \left\| H(i\omega) - \widehat{H}_r(i\omega) \right\|_2 = \left\| H(0) - \widehat{H}_r(0) \right\|_2 \overset{(10)}{\leq} \sigma_{k+1}^{I/O} + 2 \sum_{j=l+1}^{n} \hat{\sigma}_j,$$

for these circuits.

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