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Combining Krylov subspace methods and identification-based methods for Model Order Reduction

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SUMMARY

Many different techniques to reduce the dimensions of a model have been proposed in the near past. Krylov subspace methods are relatively cheap, but generate non-optimal models. In this paper a combination of Krylov subspace methods and Orthonormal Vector Fitting is proposed. In that way an optimal model for a large model can be generated. In the first step, a Krylov subspace method reduces the large model to a model of medium size, then an optimal model is derived with Orthonormal Vector Fitting as a second step.

KEY WORDS: Model Order Reduction, Krylov subspace methods, Orthonormal Vector Fitting, redundancy

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1. INTRODUCTION

In many areas of application and certainly also in the electronic industry complex simulations have to be performed. Model Order Reduction plays a vital role in keeping up with the pace of the ever increasing complexity of the simulations. Many different reduction techniques have been proposed in the near past. Two interesting methods are exposed here, Krylov subspace methods [1, 2, 3] and Orthonormal Vector Fitting [4, 5].

Krylov subspace methods are relatively cheap and can therefore handle systems with a few thousand degrees of freedom. In the meantime, the methods are known for their non-optimality: Reduced models generated by Krylov subspace methods are generally too large, since they contain information which is not needed for a good approximation.

Orthonormal Vector Fitting is an identification method, which is typically used to approximate simulated or measured frequency responses by an analytic function. Rather than reducing the state-space dimensions of a model, this technique is used to build a new model with a reduced model complexity. The goal of this algorithm is to parameterize the transfer function, such that its spectral behaviour matches the response of the larger model as accurately as possible.

In this paper a combination of both methods is proposed. In that way an optimal model for a large model can be generated. In the first step, a Krylov subspace method reduces the large model to a model of medium size, then an optimal model is derived using Orthonormal Vector Fitting in a second step.

2. KRYLOV SUBSPACE METHODS

2.1. General

Krylov subspace methods start with a state space system:

$$\mathbf{E}\frac{d}{dt}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)$$
$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t), \tag{1}$$

where $\mathbf{x}(t)$ is the state space of the system, $\mathbf{u}(t)$ is the input and $\mathbf{y}(t)$ is the output of the system. In general, $\mathbf{x}(t)$ has a very large number of entries, say n and in the case of modelling an electrical component it can consist of both voltages and currents. The system can have more than one, say p, inputs. In that case the input selecting matrix $\mathbf{B}$ has p columns.

After Laplace transforming to the frequency domain and after eliminating the state space vector $\mathbf{X}(s)$, for this system a transfer function $\mathbf{H}(s)$ can be formulated, which represents a direct relation between input $\mathbf{U}(s)$ and output $\mathbf{Y}(s)$:

$$H(s) = \mathbf{C}(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}$$

2.2. Algorithm

In Krylov subspace methods a Krylov space associated to these system matrices is generated. The definition of this Krylov space can differ. In PRIMA [2] the moments of the transfer function are collected in one space. The Krylov space is then defined as:

$$\mathcal{K}_q(\widehat{\mathbf{A}}, \widehat{\mathbf{B}}) = [\widehat{\mathbf{B}}, \widehat{\mathbf{A}}\widehat{\mathbf{B}}, \widehat{\mathbf{A}}^2\widehat{\mathbf{B}}, \ldots, \widehat{\mathbf{A}}^q\widehat{\mathbf{B}}],$$

with $\widehat{\mathbf{A}} = (\mathbf{A} - s_0\mathbf{E})^{-1}\mathbf{E}$ and $\widehat{\mathbf{B}} = (s_0\mathbf{E} - \mathbf{A})^{-1}\mathbf{B}$. In [3] the Krylov space is based on the expansion of the transfer function in Laguerre functions.

If the size of the Krylov space, pq, is smaller than the size of the system, n, a reduction can be performed by projecting the system matrices onto the Krylov space, in the following way:

$$\begin{aligned} \widetilde{\mathbf{E}} &= \mathbf{V}^T\mathbf{E}\mathbf{V} & \widetilde{\mathbf{A}} &= \mathbf{V}^T\mathbf{A}\mathbf{V} \\ \widetilde{\mathbf{B}} &= \mathbf{V}^T\mathbf{B} & \widetilde{\mathbf{C}} &= \mathbf{C}\mathbf{V} \\ \widetilde{\mathbf{D}} &= \mathbf{D}, \end{aligned} \tag{2}$$

where $\mathbf{V}$ is an orthonormal basis of the Krylov subspace. The reduced matrices then form a reduced system:

$$\begin{aligned} \widetilde{\mathbf{E}}\frac{d}{dt}\widetilde{\mathbf{x}}(t) &= \widetilde{\mathbf{A}}\widetilde{\mathbf{x}}(t) + \widetilde{\mathbf{B}}\mathbf{u}(t) \\ \widetilde{\mathbf{y}}(t) &= \widetilde{\mathbf{C}}\widetilde{\mathbf{x}}(t) + \widetilde{\mathbf{D}}\mathbf{u}(t) \end{aligned} \tag{3}$$

The transfer function of the reduced system approximates the transfer function of the original system well within a certain frequency range. It is proven that PRIMA with a Krylov subspace of order q preserves q moments of the transfer function [6]. Moreover, because of the orthogonal projection, stability and passivity are preserved [2].

Krylov subspace methods are relatively cheap. For a single point expansion, one LU-decomposition is calculated and can be reused in every iteration. The cost of an LU-decomposition is of the order n^3, the rest of the computations needed to derive the reduced model will then be $O(n^2)$. This makes Krylov subspace methods applicable to large models. Multiple input and output ports can very easily be incorporated in the reduced model, although the size of the model will increase proportionally to the number of the ports.

2.3. Redundancy

A well-known drawback of Krylov subspace methods is their redundancy: the models generated by Krylov subspace methods are in general larger than strictly needed. The iterative method tries to capture the dominant poles in quite a brute force way. Beforehand it is not known what minimal order is needed for a good approximation. Besides, there is no practical error-bound known for these methods, although an error estimate can be derived. In practice, we see that it might take long before the essential poles are approximated well. Moreover, if multiple input ports are considered it might be that the behavior of one or more ports stays behind with the rest of the ports. More iterations for these ports are needed, while an equal amount of information for all the ports is added to the space.

Quite a few propositions are published to cure this redundancy. This can either be done by a different reduction algorithm as a second step [7, 8], or by making the Krylov subspace method more efficient [9]. In [10] a way to stop the iterative process for one column while proceeding with the other ports is pointed out. Although, this partly solves the problem, the reduced models may still suffer from redundancy.

In this article we propose to combine Krylov subspace methods with Orthonormal Vector Fitting as a post-processing step.

3. ORTHONORMAL VECTOR FITTING

3.1. Algorithm

The OVF algorithm approximates the Laplace domain data samples $(s_k, H(s_k))$, $\forall k = 0, ..., K$, using a rational transfer function $R(s)$ [11]

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{p=1}^{P} c_p \phi_p(s)}{\tilde{c}_0 + \sum_{p=1}^{P} \tilde{c}_p \phi_p(s)} \quad s = i2\pi f \tag{4}$$

c_p and $\tilde{c}_p$ are the real-valued system parameters which need to be estimated, and P represents the number of poles. To obtain an improved numerical conditioning, the basis functions $\phi(s)$ are chosen to be orthonormal rational functions [12] rather than polynomials [13]. They are calculated analytically, by applying a Gram-Schmidt orthonormalization on a set of partial

fractions [14]. The orthonormality is defined with respect to the following inner product

$$\langle \phi_m(s), \phi_n(s) \rangle = \frac{1}{2\pi i} \int\limits_{i\mathbb{R}} \phi_m(s)\phi_n^*(s)ds \tag{5}$$

and the basis functions are governed by the following closed form expression

$$\phi_p(s) = \left(\prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j} \right) \frac{\sqrt{2\Re e(a_p)}}{s + a_p} \tag{6}$$

To ensure that the poles and zeros of the transfer function occur in complex conjugate pairs, the basis functions are made real-valued. This can be achieved by forming a linear combination of 2 basis functions $\phi_p(s)$ and $\phi_{p+1}(s)$ if $-a_p = -a_{p+1}^*$ [15]

$$\phi_p(s) = \left(\prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j} \right) \frac{\sqrt{2\Re e(a_p)}(s - |a_p|)}{(s + a_p)(s + a_{p+1})} \tag{7}$$

$$\phi_{p+1}(s) = \left(\prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j} \right) \frac{\sqrt{2\Re e(a_p)}(s + |a_p|)}{(s + a_p)(s + a_{p+1})} \tag{8}$$

The coefficients are estimated by minimizing Levi's cost function [16]

$$\arg\min_{c,\tilde{c}} \sum_{k=0}^{K} |D(s_k)H(s_k) - N(s_k)|^2 \tag{9}$$

Initially, the poles $-a_p$ of the basis functions are prescribed, and one coefficient (e.g. $\tilde{c}_0$) can be fixed to unity since both numerator and denominator can be divided by the same constant value without loss of generality. After simplification of (4), it becomes clear that the poles of the transfer function are essentially the zeros of the denominator. In order to calculate them, the minimal state-space realization ($\mathbf{A},\mathbf{B},\mathbf{C},\mathbf{D}$) of $D(s)$ is formed by cascading a number of smaller, first or second order sections [17]. The zeros can then easily be calculated by solving an eigenvalue problem.

$$-a_p = eig(\mathbf{A} - \mathbf{bc}) \tag{10}$$

Using a Sanathanan-Koerner iteration [18], the poles can be relocated iteratively

$$\arg\min_{c^{(t)},\tilde{c}^{(t)}} \left(\sum_{k=0}^{K} \frac{\left| D^{(t)}(s_k)H(s_k) - N^{(t)}(s_k) \right|^2}{\left| D^{(t-1)}(s_k) \right|^2} \right) \tag{11}$$

until the cost function is minimized (iteration counter t). Before each iteration, unstable poles are avoided by flipping them into the left half of the complex plane. The transfer function can

be obtained in a straightforward way by solving the residues, which is a linear problem. If the poles are stable, this can be done in the orthonormal basis

$$\arg \min_c \sum_{k=0}^{K} \left| H(s_k) - \left(\sum_{p=1}^{P} c_p^{(t)} \phi_p^{(t)}(s) \right) \right|^2 \tag{12}$$

or if unstable poles are allowed, one can resort to the partial fractions basis [19]

$$\arg \min_c \sum_{k=0}^{K} \left| H(s_k) - \left(\sum_{p=1}^{P} \frac{c_p^{(t)}}{s_k + a_p^{(t)}} \right) \right|^2 \tag{13}$$

Such representation can easily be realized as a compact RLCG circuit.

3.2. Order Estimation & Sample Distribution

3.2.1. State Space Evaluation using Adaptive Sample Distribution The goal of the OVF reduction step is to obtain a transfer function which approximates the behavior of the original system as accurately as possible, using a restricted number of poles. It is critical to select an appropriate sample distribution which captures all spectral dynamics of the original system, including resonances and coupling effects. This means that a relatively dense frequency sweep, and consequently a large amount of state-space evaluations, are required to calculate the frequency response for all elements of the system matrix.

The number of poles P_{orig} of the original system can be reduced with the Krylov method and an Adaptive Sample Distribution scheme (ASD) can be applied to obtain a good estimate of K. If the value of K is chosen too low, important effects may be missed due to undersampling. On the other hand, if this value is chosen too high, the computational cost of the state-space evaluations can be excessive. Using this ASD scheme, such problems are avoided without requiring a priori knowledge of the structure :

First an initial set of 4 equidistant data samples is selected over the frequency range of interest for each matrix element, and a rational fitting model is calculated using OVF. Between each pair of successive frequency samples, 1 or 2 additional samples are evaluated and compared to the response of the transfer function. If the deviation between the two models is too large, the sample distribution can be further refined by evaluating intermediate data points until the error is below an accuracy threshold. This approach limits the number of required state-space evaluations, and the overall computation time.

3.2.2. Model Order Estimation   Another parameter which needs to be estimated carefully is the number of starting poles P which are needed for the OVF fitting algorithm. This choice is particularly important, since the resulting transfer function will either be redundant or inaccurate if the number of poles is chosen too high or too low. Usually, one visually inspects the data, starts from an initial guess of P starting poles, which is then manually increased or decreased according to the resulting accuracy of the fitting model. During the ASD step, the number of poles was chosen sufficiently high, e.g. equal to the number of available data samples or the number of poles of the original system, depending on which value is the smallest. The order can now be reduced as follows :

1) One can start from a low number of poles, e.g. 4, in order to fit the initially selected data samples. Each time the distribution is refined, the number of poles can be gradually incremented until the accuracy in the selected data samples is sufficiently high. Rather than reducing the order of the model of the original system, this approach starts from a low number of poles which is adaptively increased as needed. Even though this method works well in practice, it does not look very appealing from a computational point of view, since this process may require a large amount of rational approximations.

2) A more efficient alternative is refit all evaluated data samples using the poles from the final rational model, which was calculated during the ASD step. These poles are relocated using the Sanathanan-Koerner iteration, and their corresponding residues are calculated. If the magnitude of the residues in the partial fraction expansion are sufficiently small, the terms with the corresponding poles can be discarded since their contribution is very limited. Based on the reduced set of poles, the poles can be relocated and discarded iteratively until the magnitude of all the residues is sufficiently large. The convergence of this method is usually relatively fast, and requires a limited number of rational approximations.

3.3. Extension to multi-port systems

The extension of OVF to multi-port systems can be done in a similar way as the matrix version of the classical Vector Fitting algorithm [19]. The basic idea is that all elements of the system matrix are stacked in one column, and are fitted using a common set of poles. This reduces to

solving the following iterative problem

$$\arg \min_{c_{ij}^{(t)}, \tilde{c}^{(t)}} \left(\sum_{k=0}^{K} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \frac{\left| D^{(t)}(s_k) H_{ij}(s_k) - N_{ij}^{(t)}(s_k) \right|^2}{\left| D^{(t-1)}(s_k) \right|^2} \right) \tag{14}$$

where H_{ij} represents the i, j^{th} element of the system matrix. The reader is referred to [19] for more implementation details. In practice, the dimensions of the system equations may become quite large, even for systems with a moderately amount of ports and poles. In fact, the number of elements in the pole identification matrix requires a large amount of memory resources and computation time. To our experience, it often suffices to select a subset of the elements of the system matrix in the pole identification step.

3.4. Passivity Enforcement

It was shown in [20], that the impedance system matrices of passive electrical networks are positive real. A square rational matrix function $\mathbf{H}(s)$, is said to be positive real if the following criteria are satisfied :

1. $\mathbf{H}(s)$ is analytic, for $\Re e(\text{s}) > 0$.
2. $\mathbf{H}^*(s) = \mathbf{H}(s^*)$
3. $\mathbf{H}(s) + \mathbf{H}^T(s^*) \geq 0$

The first and second criterion can easily be imposed by the OVF algorithm. Loosely speaking, these restrictions imply that all poles must be located in the left half of the complex plane, and that the poles and zeros of the transfer function are real, or occur in complex conjugate pairs (i.e. the coefficients of the transfer function are real). The third criterion is not satisfied in the general case, however several techniques are available to enforce this constraint a posteriori. The interested reader is referred to [21] and [22].

4. EXAMPLES

As an example we consider a planar version of a double LC-filter. The layout (and mesh) is given in Figure 1.

The quasi-static EM-behavior of this model is linear time-invariant, and can be formulated as a state space system with 695 poles and 11 ports. In Figure 2 the magnitude of the H_{11}

entry (impedance element Z_{11}) of the system matrix is given.

First we will consider only one port of the model. This single-input-single-output model corresponds with the H_{11}-element of the transfer function. We reduced the model by PRIMA to size 58. The parameter s_0 in the moment expansion for PRIMA was chosen equal to $3 \cdot 10^9$, according to the maximum frequency of interest. We define a relative error to indicate the accuracy of the approximation as follows: Let $H_{ij}(s)$ and $\tilde{H}_{ij}(s)$ be all function values of the (i,j)-entry of the original and reduced system matrix respectively, then the error is defined as:

$$e_{ij} = \max_{s} \left(\frac{\left| H_{ij}(s) - \tilde{H}_{ij}(s) \right|}{|H_{ij}(s)|} \right), \tag{15}$$

The relative error e_{11} between the original and the Krylov reduced model is then equal to $6.7 \cdot 10^{-4}$. Using the OVF method, the state-space dimensions of the reduced model can be further minimized.

Figure 3 illustrates the ASD scheme on the structure over the frequency range [1 MHz - 3 GHz]. In Figure 3(a), the algorithm starts by selecting 4 equidistant data samples, marked with circles, and builds a rational model using OVF. The approximant (dashed line) and the state-space realization of the original structure (full line) are evaluated in the intermediate data samples, which are marked with crosses. The maximum relative error is obtained by calculating the difference between these models, and it is clearly too high after the initial step. A model is built using all evaluated samples, and the density is refined as shown in Figure 3(b). Again the error is calculated in all intermediate samples, and the procedure is repeated until the error is below a given threshold, e.g. smaller than 10^{-7}. Such an accuracy $(7.5 \cdot 10^{-8})$ was obtained after running 4 iterations.

Now, the model reduction step is applied using the 2nd method (see § 3.2.2). All 244 data samples are gathered (the number of crosses in Figure 3(d)), and a rational model was build using the 82 poles which were calculated in the final iteration of the ASD step (the number of circles in Figure 3(d)). All redundant poles are discarded, based on the magnitude of their corresponding residues, and the algorithm reduces the model complexity to 31 poles in 5 SK-iterations. Table 1 illustrates the reduction of the poles per iteration, and shows its corresponding error.

The resulting accuracy in all 244 data samples is $1.5 \cdot 10^{-6}$. As a verification step, the reduced model was compared over a dense set of data samples and the overall accuracy is $3.5 \cdot 10^{-5}$. The

fitting error (i.e. the difference between the Krylov and OVF approximant) is shown in figure 4. Optionally, one can use a stepwise reduction of the number of poles as a post-processing step to further reduce the number of poles. It should be noted however that this reduction will be compensated by an increase in the fitting error.

The 695 poles of the original problem are reduced to 58 poles after Krylov reduction, and reduced to 31 poles after OVF. The overall error is bounded by $7.05 \cdot 10^{-4}$.

Now, we consider the full multiple-input-multiple-output model. The model is first reduced to size 143 by PRIMA. The maximum over all 11×11 relative errors between original and reduced model is then $4.85 \cdot 10^{-4}$.

First, it is verified by the ASD step that a sample distribution of 244 equidistant data samples is sufficiently dense. Then, each element on the diagonal of the system matrix is modeled using a set of 31 poles. The order is step-wise increased (e.g. by 1 or 2 poles) until the accuracy is sufficiently high. When the order is set to 46, the estimated accuracy of all elements is equal to $2.74 \cdot 10^{-5}$. This accuracy was verified on a very dense set of samples, and corresponds nicely to the estimate.

5. CONCLUSIONS

Krylov subspace methods, like PRIMA and Laguerre-SVD have proved to be very useful in applications where the dimensions of the state space realization are significantly large. These methods can provide a good approximation, at a relatively low computational cost. Nevertheless, the size of the reduced model will not be optimal.

Once the model is reduced to a size for which the full transfer function can be calculated in a reasonable time, the Orthonormal Vector Fitting techniques comes into play. This method is essentially an elegant combination of a Sanathanan-Koerner iteration using orthonormal rational functions [4]. Using this method, an optimal model can be easily be derived as a second step in the reduction process. This approach extends easily to multiple-input-multiple-output systems.

We have to remark that the preservation of passivity, a merit of Krylov space methods as for instance PRIMA and Laguerre-SVD is not guaranteed by OVF. Nevertheless, post-processing techniques can be applied to enforce such physical behaviour.

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6. BIOGRAPHIES

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Wil Schilders received his MSc degree in 1978 at the Katholieke Universiteit Nijmegen and his PhD in 1980 at Trinity College in Dublin. Since 1980 he is working for Philips in The Netherlands, from 1980 till 1990 in the Mathematical Software Group and since 1990 at Philips Research. His research interests are in the development of algorithms for industrial applications, especially for semiconductor problems, electronic circuits and MRI-systems.

Tom Dhaene was born on June 25, 1966, in Deinze, Belgium. He received his Ph.D. degree in Electrotechnical Engineering from the University of Ghent, Belgium, in 1993. From 1989 to 1993, he was Research Assistant at the University of Ghent, in the Department of Information

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