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 (OVF) is proposed. In that way a compact 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 a compact model is derived with OVF as a second step. Copyright © 2007 John Wiley & Sons, Ltd.

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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 [1-3] and orthonormal vector fitting (OVF) [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.

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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. This way, a large model can be reduced to a compact model. In the first step, a Krylov subspace method reduces the large model to a model of medium size, then a compact model is derived using OVF in a second step.

2. KRYLOV SUBSPACE METHODS

2.1. General

The following state-space system is considered

$$\mathbf{E}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)$$
(1)

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \tag{2}$$

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. **A**, **B**, **C**, **D** and **E** represent the state matrix, input matrix, output matrix, feedthrough matrix and descriptor matrix, respectively. In general, $\mathbf{x}(t)$ has a 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 **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 $\mathbf{Y}(s)$

$$H(s) = \mathbf{C}(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}$$
(3)

2.2. Method

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 follows:

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$$\mathscr{K}_{q}(\mathbf{A}, \mathbf{B}) = [\mathbf{B}, \mathbf{A}\mathbf{B}, \mathbf{A}^{2}\mathbf{B}, \dots, \mathbf{A}^{q}\mathbf{B}]$$
(4)

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:

$$\widetilde{\mathbf{E}} = \mathbf{V}^{\mathrm{T}} \mathbf{E} \mathbf{V}, \quad \widetilde{\mathbf{A}} = \mathbf{V}^{\mathrm{T}} \mathbf{A} \mathbf{V}$$
$$\widetilde{\mathbf{B}} = \mathbf{V}^{\mathrm{T}} \mathbf{B}, \quad \widetilde{\mathbf{C}} = \mathbf{C} \mathbf{V}$$
$$\widetilde{\mathbf{D}} = \mathbf{D}$$
(5)

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where V is an orthonormal basis of the Krylov subspace. The reduced matrices then form a reduced system:

$$\widetilde{\mathbf{E}}\frac{\mathbf{d}}{\mathbf{d}t}\widetilde{\mathbf{x}}(t) = \widetilde{\mathbf{A}}\widetilde{\mathbf{x}}(t) + \widetilde{\mathbf{B}}\mathbf{u}(t)$$
(6)

$$\widetilde{\mathbf{y}}(t) = \mathbf{C}\widetilde{\mathbf{x}}(t) + \mathbf{D}\mathbf{u}(t) \tag{7}$$

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 LUdecomposition is calculated and can be reused in every iteration. The cost of an LUdecomposition 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. It is not known beforehand 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 behaviour 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 OVF as a postprocessing step.

3. ORTHONORMAL VECTOR FITTING

3.1. Method

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

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{p=1}^{P} c_p \phi_p(s, a)}{\tilde{c}_0 + \sum_{p=1}^{P} \tilde{c}_p \phi_p(s, a)}, \quad s = i2\pi f$$
(8)

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The numerator N(s) and denominator D(s) of the transfer function are represented as a linear combination of P orthonormal rational functions [12–15], which are based on a prescribed set of poles $a = \{-a_1, \ldots, -a_P\}$. Given a set of Laplace data samples $(s_k, H(s_k))$, the coefficients c_p and \tilde{c}_p (which are the real-valued system parameters) need to be estimated such that $R(s_k) \simeq H(s_k)$, for all data samples $k = 0, \ldots, K$. The denominator has an additional basis function which equals the constant value 1. The basis functions are governed by the following closed form expression:

$$\phi_p(s,a) = \left(\prod_{j=1}^{p-1} \frac{s-a_j^*}{s+a_j}\right) \frac{\sqrt{2Re(a_p)}}{s+a_p} \tag{9}$$

if $-a_p$ is a real pole, and a linear combination of 2 basis functions is formed if $-a_p = -a_{p+1}^*$ [16]

$$\phi_p(s,a) = \left(\prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j}\right) \frac{\sqrt{2Re(a_p)}(s - |a_p|)}{(s + a_p)(s + a_{p+1})}$$
(10)

$$\phi_{p+1}(s,a) = \left(\prod_{j=1}^{p-1} \frac{s-a_j^*}{s+a_j}\right) \frac{\sqrt{2Re(a_p)}(s+|a_p|)}{(s+a_p)(s+a_{p+1})}$$
(11)

It is noted that the prescribed poles are chosen according to the following heuristical scheme

$$-a_p = -\alpha + \beta \mathbf{i}, \quad -a_{p+1} = -\alpha - \beta \mathbf{i} \tag{12}$$

$$\alpha = \beta / 100 \tag{13}$$

with imaginary parts β covering the frequency range of interest. Experimental results show that this gives the best overall results in terms of numerical robustness and convergence speed.

Levi's estimator [17] can be used to calculate the coefficients c_p and \tilde{c}_p , which corresponds to minimizing the following cost function:

$$\arg\min_{c,\tilde{c}}\left(\sum_{k=0}^{K}\left|\sum_{p=1}^{P}c_{p}\phi_{p}(s_{k},a)-\left(\tilde{c}_{0}+\sum_{p=1}^{P}\tilde{c}_{p}\phi_{p}(s_{k},a)\right)H(s_{k})\right|^{2}\right)$$
(14)

The numerator and denominator of (8) can then be factorized as follows:

$$N(s) = \sum_{p=1}^{P} c_p \phi_p(s, a) = \frac{\prod_{p=1}^{P-1} (s + z_{p,n})}{\prod_{p=1}^{P} (s + a_p)}$$
(15)

$$D(s) = \tilde{c}_0 + \sum_{p=1}^{P} \tilde{c}_p \phi_p(s, a) = \frac{\prod_{p=1}^{P} (s + z_{p,d})}{\prod_{p=1}^{P} (s + a_p)}$$
(16)

and the transfer function R(s) is easily obtained as

$$R(s) = \frac{N(s)}{D(s)} = \frac{\prod_{p=1}^{P-1} (s + z_{p,n})}{\prod_{p=1}^{P} (s + z_{p,d})} = \sum_{p=1}^{P} \alpha_p \phi_p(s, z_d)$$
(17)

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The poles $z_d = \{-z_{1,d}, \ldots, -z_{P,d}\}$ can be calculated directly as the zeros of the minimal statespace realization of D(s), so the calculation of the values for α reduces to a linear problem. In order to relocate the poles to a better position, a Sanathanan–Koerner (SK) iteration [18, 19] can be applied, using an implicit weighting scheme. This means that the coefficients $d^{(t)}$ and $\tilde{d}^{(t)}$ of the weighted numerator $(N^{(t)}/D^{(t-1)})$ and denominator $(D^{(t)}/D^{(t-1)})$ are estimated (Equation (20)), rather than the coefficients $c^{(t)}$ and $\tilde{c}^{(t)}$ of numerator $(N^{(t)})$ and denominator $(D^{(t)})$ (Equation (19)), where $w_k^{(t)} = 1/D^{(t-1)}(s_k)$

$$\arg\min\left(\sum_{k=0}^{K} \left|\frac{N^{(t)}(s_k)}{D^{(t-1)}(s_k)} - \frac{D^{(t)}(s_k)}{D^{(t-1)}(s_k)}H(s_k)\right|^2\right)$$
(18)

$$= \arg \min_{c^{(t)}, \tilde{c}^{(t)}} \left(\sum_{k=0}^{K} \left| w_k^{(t)} \left[\sum_{p=1}^{P} \frac{c_p^{(t)}}{s_k + a_p} - \left(\tilde{c}_0^{(t)} + \sum_{p=1}^{P} \frac{\tilde{c}_p^{(t)}}{s_k + a_p} \right) H(s_k) \right] \right|^2 \right)$$
(19)

$$= \arg \min_{d^{(i)}, \tilde{d}^{(i)}} \left(\sum_{k=0}^{K} \left| \sum_{p=1}^{P} \frac{d_p^{(i)}}{s_k + z_{p,d}^{(t-1)}} - \left(\tilde{d}_0^{(t)} + \sum_{p=1}^{P} \frac{\tilde{d}_p^{(t)}}{s_k + z_{p,d}^{(t-1)}} \right) H(s_k) \right|^2 \right)$$
(20)

The introduction of an implicit weighting does not pose a problem, as the zeros of $D^{(t)}$ and $D^{(t)}/D^{(t-1)}$ (i.e. the relocated transfer function poles) are equivalent. The implicit scheme, however, is numerically more reliable if the poles are not optimally chosen. The reader is referred to [4, 5] for more details about this procedure.

3.2. Order estimation & sample distribution

3.2.1. Adaptive frequency sampling (AFS). The goal of the OVF reduction step is to obtain a transfer function which approximates the behaviour of the original system as accurately as possible, using a restricted number of poles.

A uniform frequency sampling of the response often requires *a priori* knowledge about the dynamics of the structure. If the sampling is too sparse dense, undersampling may occur which results in the loss of important features of the response. Therefore, it is critical to select an appropriate sample distribution which captures all spectral dynamics of the original system, including resonances and coupling effects. On the other hand, oversampling is also undesired as it leads to a waste of computation time and resources. Even if most of the desired frequency range is oversampled, some important effects can still be missed due to local undersampling. A similar reasoning holds for the estimation of the model order. Overfitting of the structure unnecessarily increases the model complexity and complicates the enforcement of passivity, while undermodelling results in an inaccurate fitting model. Therefore, an AFS technique can be applied which adaptively selects an appropriate sample distribution and automatically converges if a desired accuracy level is reached. Such AFS algorithms minimize the computational cost of acquiring and representing observation data to a desired accuracy or uncertainty over a predefined frequency range of interest. For details, the reader is referred to [20].

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3.2.2. Simplified approach. A simplified approach consists of selecting four initial data samples which are equidistantly spread over the frequency range of interest for each matrix element. Then, a rational fitting model is calculated using OVF. Between each pair of successive frequency samples, one or two additional samples are evaluated and compared to the response of the transfer function. If the deviation is too large, the sample distribution can be further refined where needed, by evaluating intermediate data points until the error is below an accuracy threshold. The order of the transfer function can be controlled by either removing the poles from the high-order macromodel or adding poles to the low-order macromodel. In [21], the order of the model is estimated and reduced by adding poles that can be extracted from the frequency response and removing redundant poles that do not significantly contribute to the accuracy of fit. A possible decision criterion for determining redundant poles is the root-mean square (RMS) of the frequency response of the corresponding pole–residue pair over the frequency range of interest.

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 [22]. 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:

$$\arg\min_{d_{ij}^{(l)}, \tilde{d}^{(l)}} \left(\sum_{k=0}^{K} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \left| \frac{N_{ij}^{(l)}(s_k)}{D^{(l-1)}(s_k)} - \frac{D^{(l)}(s_k)}{D^{(l-1)}(s_k)} H_{ij}(s_k) \right|^2 \right)$$
(21)

where H_{ij} represents the *i*, *j*th element of the system matrix. The reader is referred to [22] for more implementation details. In practice, the dimensions of the system equations may become quite large, even for systems with a moderate 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. According to our experience, it is often sufficient to select a subset of the elements of the system matrix in the pole identification step.

3.4. Passivity enforcement

Impedance system matrices of passive electrical networks are positive real [23]. A square rational matrix function, H(s), is said to be positive real if the following criteria are satisfied:

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

The first and second criteria 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 [24, 25].

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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-behaviour 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



Figure 1. Printed circuit board layout of double LC filter.



Figure 2. The H_{11} entry of the transfer function of the double LC filter model.

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Figure 3. Fitting error between OVF (31-pole) and Krylov (58-pole) approximant.

size 58. The parameter s_0 in the moment expansion for PRIMA was chosen equal to 3×10^9 , 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

$$e_{ij} = \max_{s} \left(\frac{\left| H_{ij}(s) - \tilde{H}_{ij}(s) \right|}{\left| H_{ij}(s) \right|} \right)$$
(22)

The relative error e_{11} between the original and the Krylov reduced model is then equal to 6.7×10^{-4} . Using the OVF method, the state-space dimensions of the reduced model can be further minimized. A representative set of data samples is gathered as described in Section 3.2.2, and a rational model was build using 31 poles. The resulting accuracy in all selected data samples corresponds to 1.5×10^{-6} . As a verification step, the reduced model was compared over a dense set of data samples and the overall accuracy is 3.5×10^{-5} . The fitting error (i.e. the difference between the Krylov and OVF approximant) is shown in Figure 3.

As an example, assume that the number of poles is overestimated, like e.g. 82 poles. In this case, the redundancy of a pole–residue pair can be estimated by calculating the RMS of the frequency response. In typical cases, the magnitude of the residues of the redundant pairs is quite small in relation to the magnitude of the pole. A fitting model is calculated in five SK-iterations, and the redundant pairs are discarded in each iteration. This results that the algorithm reduces the model complexity to 31 poles in five SK-iterations. Table I illustrates the reduction of the poles per iteration, and shows its corresponding error. 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 of 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 7.05×10^{-4} .

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Iter	Poles	Fitting error
1	82	1.0056×10^{-9}
2	43	6.0139×10^{-10}
3	37	8.8089×10^{-10}
4	33	3.1227×10^{-8}
5	31	1.5122×10^{-6}

Table I. Pole-reduction using SK-iteration.

Now, we consider the full multiple-input–multiple-output (MIMO) 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 4.85×10^{-4} . Based on a representative set of data samples, each element on the diagonal of the system matrix is modelled using a common 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 2.74×10^{-5} . This accuracy was verified on a very dense set of samples, and corresponds nicely to the estimate.

5. TIMING RESULTS

This section describes some timing results which illustrate the performance of the Krylov and OVF methods. The computer code was implemented on a Pentium 4 2.66 GHz PC, in a Matlab environment. It is noted that Matlab is a non-compiled language, so the timing results are sensitive to the actual implementation. All tests in this section are performed on the 11-port Double LC model as discussed in the Examples section.

Table II shows the computation time which is required to reduce the full MIMO model, while Table III considers the computation time to reduce the H_{11} entry (impedance element Z_{11}) of the system matrix. A comparison is given in terms of the number of selected data samples, and the size of the reduced model.

It is observed that the required computation time of the OVF method (1 iteration) grows quickly, if a large amount of data samples or poles is selected. This confirms the claim that smart sampling strategies (as described in Section 3.2) are of paramount importance, especially if the number of ports is large. A known disadvantage of data-driven MOR methods (such as OVF) is that one needs to calculate the frequency response of the structure. In the general case, the computation of a single data sample may take several minutes if the state matrix A is large. On the other hand, a reduced order model can be calculated very efficiently using the Krylov method. This follows from the fact that the computation time does not grow unacceptably with the size of the reduced system. Such a model-driven MOR approach also avoids the computation of the frequency response, at the expense of redundancy in the reduced model. By combining the OVF method with the Krylov method, the state matrix is first reduced to a smaller size which is then feasible to handle with OVF. This combined approach significantly speeds up the reduction process.

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Poles	OVF, 20 samp (s)	OVF, 40 samp (s)	OVF, 60 samp (s)	Krylov (s)
101	4.2827	7.2610	14.0268	1.4022
90	2.5848	6.5392	12.6623	1.2708
79	2.2015	5.7753	10.8572	1.1594
68	1.9037	4.9247	9.5392	1.0415
57	1.7918	4.0934	7.8757	0.9440
46	1.3557	3.5157	6.4608	0.7901
35	1.0785	2.5770	4.7989	0.6808
24	0.8770	1.8277	3.4206	0.5610
13	0.6135	1.0659	1.7566	0.4350

Table II. Computation time for reduction of the MIMO system.

Table III. Computation time for reduction of single matrix element.

Poles	OVF, 20 samp	OVF, 40 samp	OVF, 60 samp (s)	Krylov (s)
57	N/A	N/A	0.3658	3.5669
46	N/A	N/A	0.3391	2.9153
35	N/A	0.3150 s	0.3300	2.2682
24	ŇA	0.3134 s	0.3210	1.6169
13	0.3058 s	0.3101 s	0.3087	0.9990

6. 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 is in general not sufficiently small.

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 (OVF) techniques comes into play. This method is essentially an elegant combination of a Sanathanan–Koerner iteration using orthonormal rational functions [4]. Using this method, a compact model can easily be derived as a second step in the reduction process. This approach extends easily to MIMO 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 are available, which can be applied to enforce such physical behaviour.

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