ARMS - Automatic Residue-Minimization based Sampling for Multi-Point Modeling Techniques

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ABSTRACT

This paper describes an automatic methodology for optimizing sample point selection for using in the framework of model order reduction (MOR). The procedure, based on the maximization of the dimension of the subspace spanned by the samples, iteratively selects new samples in an efficient and automatic fashion, without computing the new vectors and with no prior assumptions on the system behavior. The scheme is general, and valid for single and multiple dimensions, with applicability on rational nominal MOR approaches, and on multi-dimensional sampling based parametric MOR methodologies. The paper also presents an integrated algorithm for multi-point MOR, with automatic sample and order selection based on the transfer function error estimation. Results on a variety of industrial examples demonstrate the accuracy and robustness of the technique.

Categories and Subject Descriptors

B.7.2 [Integrated Circuits]: Design Aids—simulation, verification

General Terms

Algorithms, Verification

Keywords

Model Order Reduction, Multi-Dimensional Parametric Sampling

1. INTRODUCTION

It is well known in the EDA industry that the detailed models representing physical devices, obtained after the modeling and extraction steps, are in general too large for efficient simulation and verification. Reducing their order or dimension, while guaranteeing that the input-output response is accurately captured, is crucial to enabling the simulation and verification of those large systems [20].

This is the realm of Model Order Reduction (MOR). The methods for linear model reduction have greatly evolved and can be broadly characterized into two types: those based on subspace generation and projection [7, 14], and those based on balancing techniques [13, 16]. Multi-point based approaches [6, 8, 17] have recently gathered renewed attention due to their robustness and reliability. In particular, some of them [15] have been extended to tackle the issue of Parametric Model Order Reduction (pMOR), in which the system behavior depends on a set of parameters, modeling process and environmental variations, and the frequency. In this context, the multi-dimensional sample-based techniques [15], seem less sensitive to the number of parameters, and become a good alternative to the multi-dimensional moment matching approaches, [4, 11, 12, 21], which seem unable to deal with what has been denoted as the curse of dimensionality. Such techniques generate oversized models when the number of parameters and the accuracy require matching a large set of moments. However, the multi-dimensional sampling can be expensive if there is no good indication of where to place the sample points. Random based sampling can defeat the reliability of these algorithms, whereas trying to cover the complete subspace with a linear scheme is overwhelming beyond the single dimension.

In this single dimensional framework, some effort has been devoted to the sampling selection issue. Some schemes, such as Adaptive Frequency Sampling [9], are broadly applied on interpolation and rational based procedures. However these schemes start from tabulated data to build a compact model, and thus they do not take into account the data generation (i.e. to solve the system for different points), a costly issue in MOR of large systems. The work in [10] aims at automatically finding the optimal ∥H∥2 model for a fixed q-th order, based on a refinement of the interpolation points. However the algorithm can only be applied on single dimension linear systems, and needs to solve the original system at q points at each refinement iteration, which makes the procedure expensive. Resampling plans have been proposed in [18] to provide guidance for future sample point placement in linear MOR, based on variance measurements of the reduced transfer function. However, it requires the evaluation of several reduced models, which may be expensive, and, in addition, seem awkward to extend to multi-dimensional cases.

In this paper we will try to fill this gap, by proposing a novel methodology for sampling selection in single and multi-dimensional spaces. The procedure, which is directly related to the algorithm in [17], is based on maximizing the subspace spawned by the sampling set, in order to obtain a good approximation of the dominant subspace in the orthonormalization step. To avoid falling into inefficiency, the algorithm will iteratively provide a good new sample point without solving the system, and assuming no prior knowledge of the system. The method will also attempt to avoid oversampling by estimating the error on the fly, using for this the norm associated with the vectors generated. It will decide at run time whether to generate a new sample, and where to place it. Therefore, the proposed methodology will present a fully automated procedure, which will try to overcome the lack of automation in existing (sample-based) MOR procedures, and in particular in the pMOR scenario.

Although beyond the scope of this paper, the procedure is general enough to be applied to different fields, such as non-linear MOR in which the matrices exhibit non-linear dependences with the parameters or time [20] (for example, to determine suitable new trajectory
points in Trajectory Piecewise-Linear approaches [3, 19]).

The paper is structured as follows: in Section 2 an overview of the MOR paradigm is presented, along with a discussion of existing sampling schemes. In Section 3 the new scheme is introduced, along with a study of its complexity and computational issues. In this section, an efficient integration into a multi-point model order reduction algorithm is also discussed and presented. In Section 4 several examples are shown that illustrate the efficiency of the proposed technique, and in Section 5 conclusions are drawn.

2. BACKGROUND

2.1 Model Order Reduction

The main techniques in MOR are geared toward the reduction of a state space linear time-invariant system, obtained by some modeling methodology, and representing a physical system. In such representation, the output \( y \) is related to the input \( u \) via some inner states \( x \). When parametric variations are taken into account, the system is represented as a parametric state-space descriptor,

\[
C(\lambda)\dot{x}(\lambda) + G(\lambda)x(\lambda) = Bu \\
y(\lambda) = Lx(\lambda)
\]

(1)

where \( C, G \in \mathbb{R}^{n \times n} \) are respectively the dynamic and static matrices, \( B \in \mathbb{R}^{n \times m} \) is the matrix that relates the input vector \( u \) to the inner states \( x \in \mathbb{R}^n \) and \( L \in \mathbb{R}^{p \times n} \) is the matrix that links those inner states to the outputs \( y \in \mathbb{R}^p \). We assume here, as is common, that the elements of \( C \) and \( G \), as well as the states \( x \), depend on a set of \( P \) parameters \( \lambda = [\lambda_1, \lambda_2, \ldots, \lambda_P] \in \mathbb{R}^P \) which model the effects of the uncertainty. Usually the system is formulated so that the input \( (B) \) and output \( (L) \) matrices do not depend on the parameters. This time-domain description yields a frequency response modeled via the transfer function

\[
H(s, \lambda) = L(sC(\lambda) + G(\lambda))^{-1}B.
\]

(2)

The objective of pMOR techniques is to generate a reduced order approximation, able to accurately capture the input-output behavior of the system for any point in the joint frequency-parameter space,

\[
\hat{H}(s, \lambda) = \hat{L}(s\hat{C}(\lambda) + \hat{G}(\lambda))^{-1}\hat{B},
\]

(3)

where \( \hat{C}, \hat{G} \in \mathbb{R}^{q \times q} \), \( \hat{B} \in \mathbb{R}^{q \times m} \), and \( \hat{L} \in \mathbb{R}^{p \times q} \), are the reduced sets of matrices, with \( q \ll n \) the reduced order.

In general, one attempts to generate a Reduced Order Model (ROM) whose structure is as similar to the original as possible, i.e. exhibiting a similar parametric dependence allowing more control within analysis and optimization frameworks, in order to facilitate further simulations. The most common procedure to achieve this goal is to use a sensitivity-based Taylor Series Representation [4], combined with some form of orthogonal projection scheme [14].

2.2 Multi-point Projection based Approaches

Standard pMOR methodologies rely on the generation of a suitable low order subspace (spanned by the basis \( V \in \mathbb{R}^{n \times n} \)), in which the original system matrices \( \hat{C}(\lambda), \hat{G}(\lambda), B \) and \( L \) are projected. This step generates a set of new matrices \( \hat{C}(\lambda) = V^T C(\lambda) V, \hat{G}(\lambda) = V^T G(\lambda) V, \hat{B} = V^T B \) and \( \hat{L} = LV \), that define the parametric ROM.

The goal of Multi-point approaches is to generate the basis either by generating the transfer function moments from multiple expansion points \( (s_k, \lambda_k) \), or from solving the system at different sample points on the relevant frequency plus parameter space,

\[
z_a = z(s_k, \lambda_k) = (s_kC(\lambda_k) + G(\lambda_k))^{-1}B,
\]

(4)

where \( z(s_k, \lambda_k) \) is the sample vector generated at the sample point \( (s_k, \lambda_k) \), i.e. the zero order moment at that point. In this framework, the approach in [15] presents a statistical interpretation of the algorithm in [17], and enhances its applicability. In that work, the Gramian is presented in an integral form, which is numerically approximated by a quadrature scheme. The most relevant vectors among those generated by such quadrature are selected via Singular Value Decomposition (SVD) in order to build the projection matrix \( V \).

An a posteriori expected error bound, based on the study of the singular values of the SVD, can be used, with rather good results.

This approach, less sensitive to the number of parameters, is more reliable but, on the other hand, depends on a good sampling selection scheme. However, it was argued in [17] that the efficiency of the method does not depend on the "quality" of the quadrature of the integral representation of the Gramian, but on the approximation of the subspace. Regrettably, and although good results are reported with very simplistic sampling schemes, no methodology is provided for sample placement. Furthermore very little automation has been reported on pMOR methodologies, since the number of samples must be decided beforehand. Bad or poor sampling may lead to inaccurate results, whereas an excessive number of samples can lead to inefficiency.

2.3 Sample Selection Schemes

Little work has been devoted to the issue of sample selection within the framework of MOR. The authors in [10] present an iterative procedure for selecting the \( q \) best interpolation points that generate an optimal \( \|H\|_2 \) model of order \( q \). The algorithm generates \( q \) initial random samples, used to obtain a \( q \)-th order model. The eigenvalues of this reduced model are obtained (this operation is relatively cheap on the reduced model), and these eigenvalues are used as a new set of \( q \) sampling points. The procedure is repeated until the eigenvalues (i.e. next iteration sampling points) converge, generating the \( \|H\|_2 \) optimal model. However, there are some obvious drawbacks to this approach: it is only applicable on single dimensional linear systems, and it needs to solve the original system (an expensive operation) at \( q \) points on each iteration. Also, increasing \( q \) (the reduced order) implies complete model recalculation, and \( q \) has a dramatic impact on accuracy (and, of course, the required value of \( q \) for a good approximation is not known beforehand). Furthermore, the initial guess of the points is relevant in terms of the stability of the model and the efficiency, due to convergence of the eigenvalues. This means that some a priori knowledge is needed for a good initial guess.

The work presented in [18] is explicitly aimed at sample point selection for optimizing multi-point MOR schemes. There, the idea followed is to generate \( R \) ROMs of identical reduced size \( q \), resampled from the same large set, \( Z_t \ldots Z_R \), with an associated transfer function \( H_k(s) \) (with \( k = 1 \ldots R \)). If the various ROMs do not give similar results, that means that the places where the transfer functions disagree the most are likely to be good places to put a new sample point. As a metric of model uncertainty, a variance-like quantity is proposed

\[
var(s) = \frac{1}{R} \sum_{k=1}^{R} \|H_k(s) - H_{ref}(s)\|^2,
\]

(5)

where \( H_{ref} \) is the transfer function of a reference reduced model, obtained by using all the available samples (i.e. from \( Z = \cup_k Z_k \)). Points in regions with larger variance are good candidates for new sample points, and thus the procedure gives not only indication of which are the best points (and thus vectors) in the generated set, but also can guide the process of finding new sample points for generating new vectors. Although the work presents an efficient implementation to build the various ROMs and to obtain the variance, the method still has some drawbacks: one is that it requires
the evaluation of the reduced models’ frequency transfer function, and another is that it requires one to compute an initial population, i.e. an initial set of samples (and vectors) to start working with (and with no guarantee that these first samples are a good set). These issues are aggravated in multi-dimensional spaces: how to compute efficiently the multi-dimensional variance? and how to set a first sample population in this case?

3. AUTOMATIC SAMPLING PROCEDURE

This section introduces the proposed sampling scheme. As already pointed out, it is based on trying to find the minimum set of samples that will spawn a subspace that generates a good ROM.

Before presenting it, we have to set onto two basic premises. If we define $A_j = s_j C(\lambda_j) + G(\lambda_j)$, $A_{\Psi} \in \mathbb{R}^m \times n$, the system matrix for the $j$-th sampling point $(s_j, \lambda_j)$, we note that:

- To compute the system matrix for a sampling point is cheap\(^1\). We have to obtain $A_j$, and the matrices $C_j$ and $G_j$ are sparse, so the sums and products of these matrices come at a cost of $O(n^\alpha)$, with $1 \leq \alpha \leq 1.2$.

- To solve the system for a sampling point is expensive. We have to obtain the sample vector $z(s_j, \lambda_j) = A_j^{-1} B$. And thus, we must compute the $LU$ factorization of $A$, at a cost of $O(n^\beta)$, with $1.2 \leq \beta \leq 1.5$, and a set of sums and products at a cost of $O(n^\alpha)$.

This means that we should avoid computing the sample vectors $z(s_j, \lambda_j)$ unless it is strictly necessary.

It is clear that any sample will give a good vector for approximating the system, at least in the neighborhood of the point, but on the other hand, a new vector may add information that is already enclosed in the subspace generated so far (it can be well approximated by the already obtained vectors), and thus it is not a good new sampling choice. Therefore, a good new vector is one that is as much different from the ones we already have as possible, and thus, cannot be well approximated by the currently available subspace.

However, this unleashes a question: how can we determine if a candidate sample point $(s_j, \lambda_j)$ will generate a vector that adds rank to our set of vectors $Z = \{z_1, \ldots, z_k\}$ without computing it? Furthermore, how can we know if this new vector will help to minimize the number of samples needed to obtain a good ROM?

The answer is simple, we cannot. But on the other hand, we can do some simple and efficient computations that will provide a good estimate of the best candidate sample point to solve for.

3.1 Iterative Sample Selection

We start from a set $\Psi = \{\psi_1, \ldots, \psi_k\}$, in which each $\psi_j$ is a point in the space of interest. $\Psi$ is a set that covers our space of interest, and at each step, we will select from it the most appropriate point for our goals. This will be done by trying to find which point has an associated vector that is less similar to the vectors we have already computed. Although it is not a perfect indicator, this will maximize our chances of adding "relevant" rank to the subspace, and we can obtain such information in a cheap fashion.

We take the $j$-th candidate sample point, $\psi_j$, with an associate matrix $A_j = A(\psi_j)$. If we have a vector $z_j \in \mathbb{R}^n$, we can determine if it is a good solution for our system at this $j$ point by computing the norm of the residue,

$$||r_{ij}|| = ||B - A_j z_j||,$$

where $r_{ij}$ is the residue of the vector $z_j$ for the system $\{A_j, B\}$. The cost of this operation is relatively cheap since $A_j$ is sparse. If the norm is small, it means that the system $\{A_j, B\}$ is well approximated by vector $z_j$, so in this case $\psi_j$ is not a good new point.

To see if the system $\{A_j, B\}$ is well approximated by a set of vectors $Z$, we simply orthogonalize vector $B$ against the set of vectors $A_j Z$, with a resulting vector $r_j$ with an associated norm.

$$r_j = B \perp A_j Z,$$

which by itself is a measure of how close the set $A_j Z$ is to the vector $B$. A vector $B$ is well approximated by a set of vectors $Z$ if the norm of $r_j$ is small.

We can then repeat the operation for all the candidate sample points, to know, for each of them, whose solution is the worst approximated by vector $z_j$, so in this case $\psi_j$ is not a good new point.

3.2 Efficient Implementation

Some non-trivial issues arise from the computations outlined in the previous section. One is that since the operation in (7) must be repeated for each sample point in the candidate set, we are not interested in having an extremely fine set of samples covering the space under study. So how to generate the candidate set of points, and in particular how to generate it in a large dimensional space?

There is no good answer to this question, but in [18] it was shown that linear sampling is a good scheme. In addition, the PMTBR procedure is very robust, and can generate good results from small number of samples. Therefore we propose a relatively coarse linear mesh, covering the space of interest. A finer mesh may provide better candidates, and thus a final more compressed model, but on the other hand would increase the complexity of the model generation. Also, there is nothing to prevent us from adding new sample points to $\Psi$ at a later stage (or even on the fly) if we determine that a certain region is under-represented in the set.

Another issue is when to stop looking for new samples. In this case, the answer is simple: when the latest generated vector does not add rank. An efficient method for obtaining such information

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\(^1\)we envision the application of AMRS in conjunction with an extraction methodology that provides variational information $[1, 5]$, which makes $A_j$ evaluation for different parameter settings inexpensive.
is not degraded (to add new vectors to a which needs to be 6 samples, and placement of the 11, 12, 13 and 14-th points respectively.

is to use an incremental QR decomposition, for example a Rank Revealing (RR) QR [2]. Every time a new sample vector is generated, orthonormalize it against the already orthonormalized set of vectors, and check its norm against the tolerance desired. It must be noticed that although not a perfect indicator, this tolerance is correlated with the error, and can be used to automate the procedure. This step can be integrated with the sampling scheme into a complete multi-point MOR projection based algorithm, as the orthonormalized set of vectors provides the basis of the subspace into which the matrices are going to be projected. Algorithm 1 gives a more clear depiction of the complete methodology.

The last issue is related to the applicability on multiple-input multiple-output (MIMO) systems. Let us take the case in which \( B = L^T \), i.e. all the inputs are also outputs of the system, for simplicity, and without loss of generality. It is important to notice that the procedure tries to find new points for which the available subspace does not provide good approximations. This can be extrapolated to the MIMO case in a straightforward manner. The only difference is that in (7), \( B \) and \( r_j \) are matrices with \( m \) \( m \) the number of inputs) columns. The norm must be obtained for a matrix instead for a vector, which is slightly more expensive, but on the other hand each step generates \( m \) new vectors, that maximize the subspace growth, and thus fewer samples will be required.

3.3 Weighted Approaches

Some applications may require different levels of accuracy in different regions of the sampling space. For example, some regions may be characterized in detail, whereas other regions may not need a very fine approximation. This can be easily achieved with the proposed methodology by controlling the sample population used. For example, let us assume we have an \( I \) region \( \Psi_{I} \) in which we desire a fine approximation, and a \( II \) region \( \Psi_{II} \) which needs to be coarsely approximated. We can then use the procedure on a candidate set that covers the \( I \) region, with a small tolerance, to generate a good model in such region. Once this model is generated, we add the samples of the candidate set that covers the \( II \) region. Then the methodology can be applied with this new set, with a less strict tolerance, in order to upgrade the model generated in the first step to obtain a coarse accuracy in the new region \( II \), while ensuring that the accuracy in region \( I \) is not degraded (to add new vectors to a basis will not degrade the ROM’s existing accuracy).

This weighting scheme can be used in parametric approaches, where the more probable region of the parameters are covered using an initial \( \Psi \) set. Once this region is well approximated, points belonging to less probable regions can be included in the remaining set, and this can be used to refine the first obtained model. This procedure also allows us to reduce the number of samples in the candidate set every time the algorithm is applied: less probable regions can be coarsely populated with a smaller number of points in the candidate set. This will lead to better efficiency, although it may degrade the optimality of the sample selection, since we are not taking into account the complete domain, and thus are selecting new samples based on a local criterion.

4. SIMULATION RESULTS

In this section we present the capabilities of the proposed algorithm (denoted as ARMS) for multiple different benchmarks. For comparison, we will use a PMTBR approach based on other sampling schemes. In the single dimensional case (frequency), uniform sampling will be used. For the multi-dimensional (parametric) cases, a pure random and a pseudo-uniform sampling will be used. The pseudo-uniform sampling consist in covering the frequency range with uniform samples (i.e. with zero variation), and around each of those samples take a set of parametric random samples. As benchmarks we will use two examples depending solely on the frequency, and two parametric systems. The first (denoted as Ex-A) is a well known 304-states PEEC example, which has already appeared in the literature [7], and which has very sharp resonances. The second (Ex-B) is a frequency dependent example obtained with an RCK-based EM extraction method. It corresponds to a strip-line whose model has 9172 states. The third (pEx-C) is a 334-states parametric RLC system obtained from an industrial
In this section we demonstrate the capabilities of our point selection method, and the fast convergence to a good solution of the proposed methodology. In Figure 1 we show a set of consecutive sample points automatically selected by the ARMS algorithm, without any knowledge of the system, and an initial population of 100 candidate samples between the minimum and maximum frequencies. The figure shows, for the Ex-B example, the transfer function absolute error with respect to the original system for a given number of consecutive samples and, marked with a star, the frequency where ARMS is going to place the next sampling point. We can see that the selection points are placed in regions of large error, or in regions in which the sample will significantly reduce the overall error. Next, in Figure 2 we show the convergence of the error in the transfer function versus the number of samples for Ex-A and Ex-B examples. It can be seen that the models generated with ARMS exhibit a faster convergence of the error. In the case of multi-dimensional environments, we show the same plot in Figure 3 for the pEx-C example, with the results of pure random, pseudo-uniform sampling (denoted as uniform) and ARMS methodologies. The results are obtained from a Monte-Carlo (MC) simulation with 159720 evaluation points finely covering the complete space of interest. The convergence of the error in the ARMS approach is much faster even in this relatively simple test case.

Figure 4: Ex-A: Transfer function and relative error w.r.t. the original system, for the proposed ARMS procedure, and the uniform sampling, with the same number of samples (note the scale on the Y-axis). ARMS sample points are also shown.

Figure 5: Ex-B: Transfer function and relative error w.r.t. to the original system for the proposed ARMS procedure, and uniform sampling, with the same number of samples. ARMS sample points are also shown.

4.2 Algorithm Accuracy and Automation

In this section we discuss the algorithm’s features in terms of accuracy and automation. For the non-parametric systems, the ARMS algorithm will be compared against a uniformly sampled PMTBR. It is important to notice that the comparison is not fair (to our disadvantage), since the uniform PMTBR approach needs to know the number of samples beforehand, whereas the ARMS approach does the selection of the number and placement of the samples at run time. For ARMS, we only fix the minimum and maximum frequencies, and the tolerance. The reduction with PMTBR is done with the same number of samples reported by the ARMS method, and with the same tolerance. First we show the transfer functions and error for ARMS and PMTBR, versus the original response, for the non-parametric examples (Ex-A and Ex-B), in Figures 4 and 5 respectively. In all cases the accuracy is very good, and the responses of the original and ROM models appear indistinguishable, but the sample points selected by the ARMS procedure (also shown) are placed in regions of large variation of the transfer function, or near sharp resonances, yielding a more accurate model than the PMTBR approach. Figure 6 shows the absolute error versus the tolerance given by the ARMS algorithm for the Ex-A and Ex-B examples. It can be seen that although there is not a perfect match, the tolerance gives a good estimator of the error. Figure 7 shows the relative error distribution for the more complex parametric pEx-D benchmark. Results are shown for the Variational PMTBR based on Pseudo Uniform and Random sampling, and for the proposed ARMS algorithm. Notice that the X-axis scale is the same. For the same number of samples, the ARMS methodology outperforms the other methodologies. In this more complex case, in which the parameters have very different range of variations, ARMS provides a better guidance for sample selection. Notice that the deviation around the mean error is much smaller in the ARMS case. This is a good indicator that the procedure selects new samples in the areas of larger error, in order to minimize the maximum.
Figure 6: Maximum absolute error $|H_e - H|$ versus the tolerance given to the ARMS algorithm, for Ex-A and Ex-B.

Figure 7: pEx-D: Distribution of the Relative error from an MC simulation with 7700 evaluation points in the space of interest, for (Top) Random sampling, (Center) Uniform sampling, and (Bottom) ARMS.

5. CONCLUSIONS

This paper presents an efficient algorithm for automatic selection and minimization of the number of samples to use in a MIMO multi-point MOR framework. The methodology, based on maximizing the spanned subspace, iteratively provides new sample points. It is general and hence easily applicable to multi-dimensional problems. The procedure was also integrated into an efficient MOR algorithm that controls the number of samples generated, and provides a good convergence of the error. It was shown that it offers a reliable, robust and accurate framework able to deal with different cases. Results demonstrate that it outperforms other sampling schemes both in single and multiple dimensions.

6. REFERENCES


