Passivity-Based Sample Selection and Adaptive Vector Fitting Algorithm for Pole-Residue Modeling of Sparse Frequency-Domain Data

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ABSTRACT

In this paper, an adaptive sampling and modeling technique is presented for accurate broadband modeling of highly dynamic systems, based on a sparse set of support samples. The method is numerically more stable than conventional approaches, while desired physical properties such as system stability, causality and even passivity can be imposed. The algorithm adaptively selects a quasi-optimal sample distribution and model complexity. During the modeling process, no prior knowledge of the system's dynamics is used.

1. INTRODUCTION

Accurate simulation of complex multi-port LTI systems can be computationally very expensive and resource-demanding, which is the case for full-wave EM simulations. One often wants to minimize the number of costly data samples, in order to find an accurate broadband model in an acceptable amount of time. In the past, several adaptive frequency sampling algorithms were presented. Traditionally, the Rational Linear Least Squares technique (RLLS) is used to calculate the coefficients of the rational model by solving a Vandermonde-like system of equations. The conditioning of this system deteriorates fast when the order of the model increases, or when the frequency range of interest gets quite broad [1]. Is it well known that reformulating the numerator and denominator polynomial as a linear combination of Chebyshev orthogonal polynomials of the first kind [2] improves the numerical issues. The large variations of Chebyshev polynomials make it possible to downsize the effects of the ill-conditioned matrix, by summing the orthogonal Chebyshev polynomials instead of summing the powers of s, which show little variation with increase in order [3]. It is always possible to convert a continuous orthogonality relationship into a discrete orthogonality relationship simply by replacing the integral with a summation. Also, the inner product can be defined on a discrete data set. The decomposition of numerator and denominator polynomial in a Generalized Formal Forsythe Orthonormal basis can be used to further improve the conditioning of the set of normal equations [4][5]. To model highly dynamic systems, which require large state-space dimensions, the former techniques can be combined with the use of splines [6]. However, for scattered deterministic data, interpolation techniques can provide a good solution as well. In [7], interpolation with Thiele-type branched continued fractions was used for this application. A tableau of quantities similar to Newton's divided differences is generated from which the coefficients are gathered to obtain an interpolating rational expression. The interpolant is recursively expanded, reaching a convergent value when all new support points are selected. Similarly, recursive algorithms of the Neville-type can be used, although they are less efficient when a large number of function evaluations are required, or if the model coefficients are explicitly needed [8]. Of course, when computing a univariate rational interpolant, both interpolation methods provide the same rational model, essentially because they all solve the same interpolation problem. Although both methods provide very accurate solutions, they often fail when the data is contamined with noise.

In this paper a new adaptive algorithm will be presented that avoids most of these problems. An iterative least-squares pole-residue modeling technique (called Vector Fitting [9]) will be used, that starts with an initial set of poles. In successive steps, the poles are relocated and the residues are calculated to optimize the fit. This way, each stage of the algorithm reduces to a linear problem. This approach provides more robust results compared to other least-squares methods, while enforcing desired physical properties such as system stability and causality.

To avoid instabilities in the time domain, the macromodels are often required to be passive. In [10], constraints are imposed on the model which are sufficient but not necessary, and therefore may lead to an undesired loss in accuracy. Other techniques such as [11] provide a set of passivity constraints which are necessary but not sufficient, hence they provide models which can still obtain small passivity violations. Usually, the latter is combined with techniques which are suited for small passivity violations, based on spectral perturbation of Hamiltonian matrices [12] or perturbation of the residues [13]. However, the quality of the model after

such post-processing techniques is often highly dependent on the quality of the model prior to the enforcement. Therefore, it will be shown that adaptive sampling strategies can minimize passivity violations within the frequency range of interest during the modeling process, while maximizing the correspondence of the model to the simulated data.

2. VECTOR FITTING ALGORITHM

In [9], a new robust iterative fitting technique, called Vector Fitting (VF), was introduced that builds accurate pole-residue models, based on frequency domain data samples. The technique is stable and resolves most of the numerical issues, encountered by other techniques. All elements of the state-space matrix are modeled by a rational pole-residue model, based upon a common set of support samples.

$$S(j\omega_i) = \sum_{n=1}^{N} \frac{c_n}{j\omega_i - a_n} + d + j\omega_i h \qquad (1)$$

$S(j\omega_i)$ represents the data samples simulated at the discrete complex frequencies $j\omega_i$, $\forall i = 0, ..., K$. a_n and c_n are the poles and residues respectively, $\forall n = 1, ..., N$. d is a constant and h is a linear factor.

The Vector Fitting technique linearizes the non-linear identification problem by fixing the denominator. It starts with an initial set of K poles, and converges towards a global broadband solution in an iterative way by relocating the poles. The unknown system variables are estimated by solving 2 linear least-squares fits, and it is imposed that the poles and residues are real or occur in complex conjugate pairs. To enforce Bounded-Input-Bounded-Output (BIBO) system stability, unstable poles are flipped into the left half of the complex plane.

3. ADAPTIVE SAMPLING

In order to have a "good" approximation of the system, it is important that all coupling effects, resonances and via's are modeled accurately. Since no prior knowledge of the system is assumed, a possible approach is to select a set of support samples which are uniformly distributed over the frequency range of interest. Although this method can be useful when the data is cheap to simulate, it can be computationally expensive and resource demanding when the simulation of data samples is costly. Reducing the spectral density of the data samples can be an option when the data behaves smoothly, however a higher accuracy of the model is obtained if the samples are selected more optimally with adaptive sampling techniques [5]. These techniques automatically select a quasi-optimal sample distribution, and an appropriate model complexity .

Figure 1 shows the best fitting model of a Lowpass Filter when 21 samples are selected equidistantly spread over the frequency range of interest (2-6 GHz). Figure 2 shows the best fitting model of the same example, with adaptively selected samples. Clearly, the adaptive technique obtains a much higher accuracy (3 significant digits) compared to the uniform distribution (1 significant digit), using the same amount of simulation time.

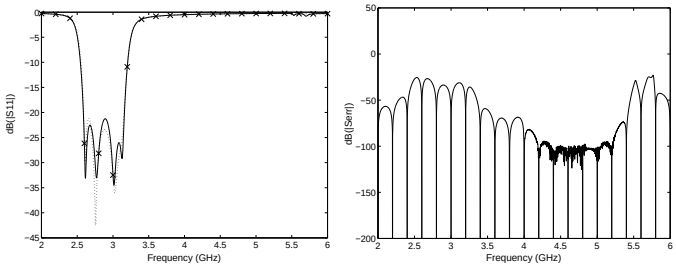

Figure 1: Magnitude Lowpass filter (full line) and fitting model (dotted line) with uniform sampling distribution at left. Complex error between fitting model and verification data at right. Accuracy fit : -22.9730 dB

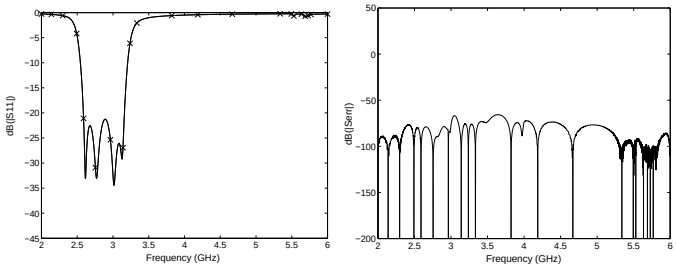

Figure 2: Magnitude Lowpass filter (full line) and fitting model (dotted line) with adaptive sampling distribution at left. Complex error between fitting model and verification data at right. Accuracy fit : -65.6536 dB

The flow chart of the algorithm is shown in Figure 3. It consists of an adaptive modeling loop, and an adaptive sample selection loop. The goal is to minimize the error of the fitting model according to the following error criterium

$$dB(|S_{ref}(j\omega) - S_{fit}(j\omega)|) < -60 \qquad (2)$$

The algorithm starts with 4 samples equidistantly spaced over a certain frequency range of interest. Depending on the number of available data samples, multiple rational models are built with different order of numerator and denominator, exploiting all degrees of freedom. All rational fitting models are evaluated in the data points, and compared against

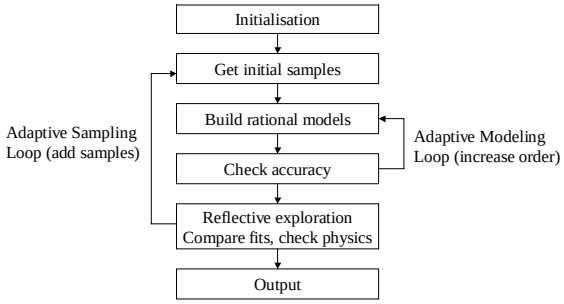

Figure 3: Flowchart of the Adaptive Sampling and Modeling Algorithm

one another. If the error between the model, evaluated in the selected sample points and the simulated data samples exceeds a certain threshold, the model is rejected, and the model's complexity is increased. All models with different order of numerator and denominator are ranked, and the 2 best models (i.e. with lowest overall error) are retained. The difference between these 2 models is called the estimated fitting error, and new samples should be chosen in such way, that the maximum estimated fitting error is minimized.

Note that the estimated fitting error is always an estimation of the real error, as this would only be known after performing a lot of computationally expensive verification simulations. Although the estimated fitting error provides a good measure to determine the frequency where the uncertainty of the model is maximal, it can sometimes cause the algorithm to converge prematurely. A good way to increase the reliability of the method, is to combine this estimated fitting error with a heuristic engine. Each time new models are generated, the algorithm checks the heuristic rules, and terminates when they are all satisfied.

Such rules, called *reflective functions* [14], compare

- Correspondance of the phase
- Correspondance of the magnitude
- Correspondance of the Euclidean distance in the complex plane

between

- Fitting model and simulated data samples
- Fitting models, calculated from overdetermined set of equations (approximants)
- Fitting models, calculated when all interpolation conditions are satisfied (interpolants)
- Fitting models, based on a different set of support samples
- Fitting models, based on a subset of selected support samples
- Fitting models, based on neighbouring and overlapping frequency ranges

while detecting

- Passivity violations
- Other unphysical effects

4. PASSIVITY CONSIDERATIONS

To avoid instabilities in the time and frequency domain, the macromodels are required to be passive. In this paper, we will focus mainly on scattering representations of the data, but a similar reasoning holds in the case of hybrid representations. For more detailed information, we refer the reader to [12][13].

Definition 1 : A system with scattering matrix $S(j\omega)$ is *passive* if the transfer function is bounded real

$$I - S(j\omega^*)S(j\omega) \geq 0 \quad \forall\omega \tag{3}$$

which is equivalent to

$$\max(\sigma(S(j\omega))) \leq 1 \quad \forall\omega \tag{4}$$

where $\sigma(S(j\omega))$ represent the singular values of S at complex frequency $j\omega$.

Definition 2 : A system with scattering matrix $S(j\omega)$ is *asymptotically passive* if (4) is satisfied for $\omega \to \infty$

In [5], only gain-violations were checked at a fixed set of discrete frequencies, to check the model for unphysical effects. However, the reliability of this technique depends mainly on the density of the sweep and can be computationally expensive, which is not desired. More accurate results are obtained when regions of passivity violations are determined algebraïcally, using the eigenvalues of the Hamiltonian matrix H. In [15], some theorems are introduced. Hereby, we assume that $S(j\omega)$ has no poles on the imaginary axis.

Theorem 1 : A system $S(j\omega)$ is passive $\Longleftrightarrow$ the Hamiltonian H has no imaginary eigenvalues.

$$H = \begin{pmatrix} A - BR^{-1}D^TC & -BR^{-1}B^T \\ C^TQ^{-1}C & -A^T + C^TDR^{-1}B^T \end{pmatrix} \tag{5}$$

where

$$Q = DD^T - I \quad (6)$$
$$R = D^T D - I \quad (7)$$

provided that Q and R are non-singular. A,B,C,D are the state-space equation representation matrices of $S(j\omega)$.

The converse also holds. A strictly stable system $S(j\omega)$ is not passive $\Longleftrightarrow$ H has imaginary eigenvalues.

Theorem 2 : $1 \in \sigma(S(j\omega_i)) \Longleftrightarrow j\omega_i$ is an eigenvalue of H

A formal proof of these theorems can be found in [15].

Using these 2 theorems, it is straightforward to detect the boundaries of passivity violations. After calculating the slopes of the singular value curves at these frequencies, an eigenvalue sweep on the sign of these slopes provides the exact regions of passivity violations [12].

If the passivity violations are sufficiently small, these defects can be resolved by spectral perturbation of the Hamiltonian matrix or perturbation of the residues. However, the quality of the model after such post-processing techniques is often highly dependent on the quality of the model prior to the enforcement. The smaller the passivity violations, the easier it is to correct the behaviour. By taking care of the passivity conditions during the modeling process and adaptive sample selection, the overall model quality can be improved right from the start. This approach can be applied until the maximal passivity violation within the frequency range of interest is below a given threshold, and small enough to be resolved with first-order matrix perturbations or other techniques.

This check can also be used in the heuristic engine as a reflective function, since it provides additional information to the sample selection and convergence detection process (see Example 1).

Therefore, additional samples are selected at complex frequency $j\omega$ within a passivity violation region $[\omega_k, \omega_{k+1}]$ where

$$\max(\sigma(j\omega)), \forall\omega \in [\omega_k, \omega_{k+1}] \quad (8)$$

is maximal until

$$\max(\sigma(j\omega)) < \varepsilon, \forall\omega \in [\omega_0, \omega_K] \quad (9)$$

Using the bisection method, the optimum can be found quite easily with minimal computational overhead.

5. EXAMPLE 1 : BANDPASS FILTER

To illustrate the presented technique, a one-port Bandpass filter was modeled over the frequency range [0.02 GHz - 1.00 GHz]. All data samples are simulated with the planar full-wave electro-magnetic simulator Agilent EEsof Momentum [16]. The desired model accuracy of the S-parameters is -60dB or better, which corresponds to a maximal error on the magnitude of 0.001. For the sake of illustration, only samples are selected at frequencies were unpassive behaviour was detected. In reality, this is only one criteria of the heuristic engine.

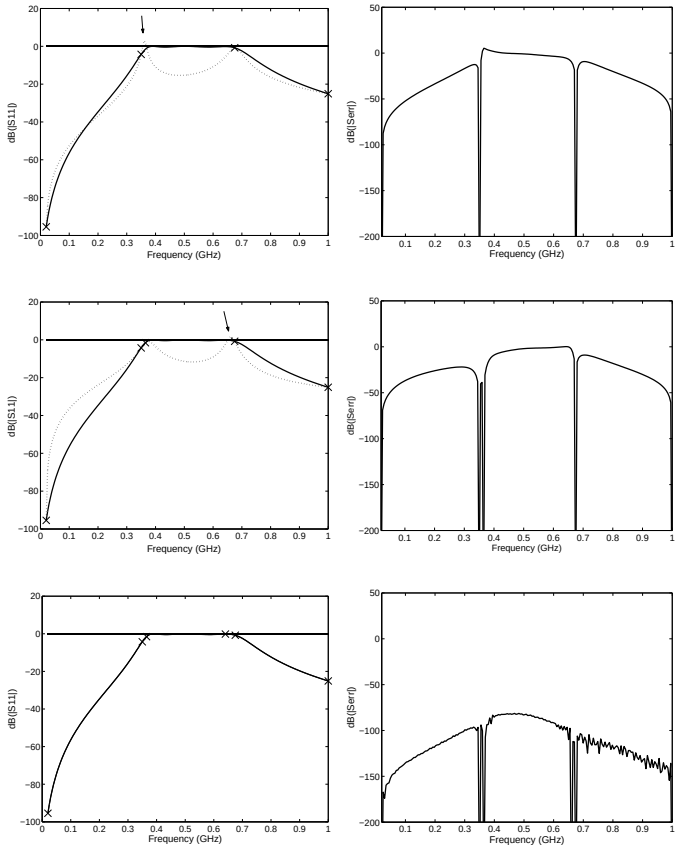

Figure 4: Illustration of each step of the algorithm (when 4, 5 and 6 samples are selected). Magnitude Bandpass filter (full line) and best fitting model (dotted line) at left. The real fitting error at right. Accuracy fit : -82.4049 dB

In order to detect the regions of unpassive behaviour, we calculate in each step the eigenvalues of the Hamiltonian matrix. After extracting the eigenvalues on the positive part of the imaginary axis, we can pinpoint the exact locations of the passivity violation, and select a new sample where the maximum violation is found. As an illustration, the eigenvalues are shown below, and the boundaries of these regions are marked with an arrow. Note that quite often, there is a significant correspondence between this maximum and the frequency where the real error is maximal. The

consecutive steps of the algorithm are shown in Figure 4, each time when an additional sample is selected.

```
Eigenvalues Hamiltonian matrix (4 samples):

+0.00000000000000 - 0.35556635157541i
-0.00000000000000 - 0.36797493144273i
-0.00000000000000 + 0.35556635157541i <--
+0.00000000000000 + 0.36797493144273i <--
+0.00920677614147 - 0.67657524224380i
+0.00920677614147 + 0.67657524224380i
-0.00920677614147 - 0.67657524224380i
-0.00920677614147 + 0.67657524224380i

Violation : [0.3555663,0.3679749] GHz

Eigenvalues Hamiltonian matrix (5 samples):

+0.00000000000000 - 0.65156791824123i
-0.00000000000000 - 0.67230698556846i
-0.00000000000000 + 0.65156791824123i <--
+0.00000000000000 + 0.67230698556846i <--
+0.19217333633158 + 0.00000000000000i
-0.19217333633158 + 0.00000000000000i
+0.01014688998501 - 0.37471499581693i
-0.01014688998501 - 0.37471499581693i
+0.01014688998501 + 0.37471499581693i
-0.01014688998501 + 0.37471499581693i

Violation : [0.6515679,0.6723069] GHz

Eigenvalues Hamiltonian matrix (6 samples):

+0.00539549345271 - 0.38963154992961i
-0.00539549345272 + 0.38963154992961i
-0.00539549345272 - 0.38963154992962i
+0.00539549345272 + 0.38963154992961i
-0.00677392820199 - 0.50292408510574i
-0.00677392820201 + 0.50292408510575i
+0.00677392820199 - 0.50292408510573i
+0.00677392820201 + 0.50292408510572i
+0.01921270798832 - 0.64595773831741i
+0.01921270798832 + 0.64595773831741i
-0.01921270798832 - 0.64595773831741i
-0.01921270798832 + 0.64595773831742i

Violation : None
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In the case of Single-Input-Single-Output, there is only one singular value curve, which corresponds to the magnitude of the data. Once 6 samples are selected, the desired accuracy of -60dB was reached, and the algorithm terminates. Although in this example the system is globally passive, this is not necessarily always guaranteed.

6. EXAMPLE 2 : QUARTER WAVELENGTH

To illustrate the numerical robustness of the technique, the entire system matrix of a 2-port Quarter Wavelength filter was modeled over the frequency range [1 GHz - 12 GHz]. The desired model accuracy of the S-parameters is -60 dB, and the maximum threshold for the singular value curves was set to 1.001. The use of a threshold is required, since ringing effects may occur when some samples are clustered around a certain frequency. In this example, we use the full heuristic engine. The final results are shown in Figure 5.

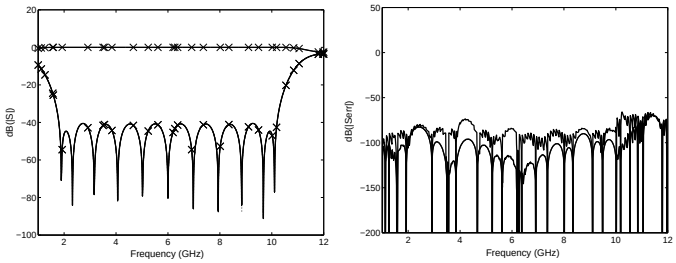

Figure 5: Magnitude data from different ports Quarter Wavelength filter (full lines) and fitting models (dotted lines) at left. Real error of all fitting models at right. Selected samples are marked with a cross. Accuracy fits : -65.9112 dB

The algorithm terminates when 30 samples are selected. The accuracy of the model and the maximal passivity violations are below the predefined thresholds.

7. CONCLUSIONS

A numerically robust Adaptive Sampling and Modeling technique was presented, that generates accurate and stable broadband pole-residue models. The use of Vector Fitting avoids most of the numerical issues, which are encountered with other least-squares fitting techniques. The algorithm adaptively selects a minimal set of support samples and converges without any prior knowledge of the system's dynamics. It avoids oversampling and undersampling, as well as overmodeling and undermodeling. During the modeling process, passivity violations within the frequency range of interest are minimized.

8. ACKNOWLEDGMENTS

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