Accurate Multi-point Padé Approximation of Microwave Structures using Orthonormal Polynomial Basis Functions

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Abstract

Rational least-squares techniques are commonly used to build compact macromodels of passive microwave components. This paper describes a technique which calculates rational least-squares fitting models by matching S-parameter frequency data-samples and higher-order frequency derivatives (or moments), using orthonormal polynomial basis functions to improve the numerical accuracy. Some considerations are given about the optimal choice of polynomial basis functions.

1. INTRODUCTION

Rational least-squares techniques are often used to calculate rational fitting models by approximating the scattering parameter matrices of passive electrical and electronical components.

Solving the approximation problem in a traditional monomial power series basis leads to ill-conditioned Vandermonde-like systems of equations which are hard to solve in finite machine precision. In [1] and [2], it was shown that orthonormal polynomials, generated by a symmetric Lanczos process can lead to an improvement in numerical conditioning.

This paper shows how frequency derivatives are included in the fitting process. A possible application is the matching of moments at multiple expansion points, which is widely recognized as a useful tool in the context of Reduced Order Modeling (ROM). Also, frequency derivatives can provide additional information to adaptive sampling techniques, which are often used to model deterministic simulation-based data at a reduced computational cost.

Finally, the optimality of the technique is discussed, and some considerations are given about alternative polynomial basis functions which can further improve the numerical accuracy of the technique.

2. RATIONAL APPROXIMATION

2.1 Rational model

A rational model $R(s)$ is defined as a quotient of two polynomials $N(s)$ and $D(s)$

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n=0}^{N} N_n s^n}{\sum_{d=0}^{D} D_d s^n} \qquad s = j2\pi f \qquad (1)$$

where N and D represent the order of numerator and denominator respectively, and N_n and D_d the polynomial coefficients. The rational function provides an approximation of the spectral response of the system over the interval $[f_{\min}, f_{\max}]$. Since there are N+D+1 unknown coefficients (D_0 can be chosen arbitrarily, e.g. D_0=1), a set of K=N+D+1 samples (s_k,$H(s_k)$) is required to identify $R(s)$ completely. $R(s)$ is then an interpolating curve passing through the values $H(s_k)$ at the complex frequencies s_k, for k=1,…,K.

To estimate the polynomial coefficients in a least squares sense, the following non-linear cost function needs to be minimized

$$\arg\min_{N,D} \sum_{k=1}^{K} \left| R(s_k) - \frac{\sum_{n=0}^{N} N_n {s_k}^n}{\sum_{d=0}^{D} D_d {s_k}^d} \right|^2 \qquad (2)$$

Due its non-linear nature, this optimization problem is often replaced by a linearized variant, e.g. using Kalman's method [3][4].

$$\approx \arg\min_{N,D} \sum_{k=1}^{K} \left| \sum_{d=0}^{D} D_d {s_k}^d R(s_k) - \sum_{n=0}^{N} N_n {s_k}^n \right|^2 \qquad (3)$$

Both methods are essentially different, however the linearized problem is commonly used in Engineering, and often provides acceptable results in practice. If not, one can resort to the use of non-linear optimization techniques, or e.g. the use of iterative least-squares techniques, such as a

Sanathanan-Koerner iteration [5]. A more detailed analysis is beyond the scope of this work.

In some cases, it's possible to obtain t^{th} order frequency derivatives $(s_k, H^{(t)}(s_k))$ from the simulator. Frequency derivatives are scaled moments (coefficients of the Taylor series at a given expansion point), which can often be simulated at a significantly lower computational cost than data samples. Taking them into account can significantly reduce the overall simulation cost, since they provide additional information to the modeling process [6].

2.2 Orthonormal polynomial bases

Let's define matrix V and vector H as

$$V_r = [s_1^r \; s_2^r \; \ldots s_K^r]^T \text{ and} \tag{4}$$

$$H = diag(H(s_1),\ldots,H(s_K)) \tag{5}$$

Then the identification problem can be formulated in terms of the unknowns $N=(N_0\ldots N_N)^T$ and $D=(D_1\ldots D_D)^T$ as

$$\begin{pmatrix} V_{0:N} & -HV_{1:D} \end{pmatrix} \begin{pmatrix} N \\ D \end{pmatrix} = \begin{pmatrix} HV_0 \end{pmatrix} \tag{6}$$

The columns of the Vandermonde matrix V are $[1, S1, S^2 1, \ldots, S^r 1]$, where $S=\text{diag}([s_1,s_2,\ldots,s_K])$, and 1 is a K column vector with all entries set to 1. Hence, the columns of V form a Krylov subspace $K_{r+1}(S,1)$. Since S is symmetric, an orthonormal basis is calculated using a symmetric Lanczos method, which produces the factorization $SQ=QT$ [7]. It follows that Q has orthonormal columns which span $K_{r+1}(S,1)$, and T is tridiagonal. Based on the elements of T, the polynomial basis is defined by a three-term recurrence relation

$$p_i(s) = \left(\frac{s - t_{i,i}}{t_{i+1,i}}\right) p_{i-1}(s) - \frac{t_{i-1,i}}{t_{i+1,i}} p_{i-2}(s) \tag{7}$$

To obtain polynomials which satisfy complex conjugate symmetry, it is required that the basis polynomials are orthonormal on both sides of the frequency axis. This corresponds to generating $\widetilde{K}_{r+1}(\widetilde{S}, \widetilde{1})$ where $\widetilde{S}=\text{diag}([s_1,\ldots,s_K,s_1^*,\ldots,s_K^*])$, $\widetilde{H}=\text{diag}(H,H^*)$ and $\widetilde{1}$ is a 2K column vector with all entries set to 1. In practice a similar result is obtained by using a modified Arnoldi process where only the real projections are used. This way, the orthonormal polynomial basis is defined by a simplified three-term recurrence relation ($\widetilde{t}_{i,i}=0$).

$$p_i(s) = \frac{s}{\widetilde{t}_{i+1,i}} p_{i-1}(s) - \frac{\widetilde{t}_{i-1,i}}{\widetilde{t}_{i+1,i}} p_{i-2}(s) \tag{8}$$

So, the coefficients of the rational model

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n=0}^{N} N_n p_n(s)}{\sum_{d=0}^{D} D_d p_d(s)} \tag{9}$$

are calculated in the orthonormal basis [1][2][8] by solving

$$\begin{pmatrix} \widetilde{Q}_{0:N} & -\widetilde{H}\widetilde{Q}_{1:D} \end{pmatrix} \begin{pmatrix} N \\ D \end{pmatrix} = \begin{pmatrix} \widetilde{H}\widetilde{Q}_0 \end{pmatrix} \tag{10}$$

2.3 Frequency Derivatives

When frequency derivatives of the data are available, the orthonormal polynomials can be generalized.

$$p_i^{(t)}(s_k) = \frac{t p_{i-1}^{(t-1)}(s_k) + s p_{i-1}^{(t)}(s_k) - \widetilde{t}_{i-1,i} p_{i-2}^{(t)}(s_k)}{\widetilde{t}_{i+1,i}} \tag{11}$$

Hence, the coefficients N_n and D_d of the rational fitting model now satisfy

$$H^{(t)}(s_k) \sum_{d=0}^{D} D_d p_d^{(0)}(s_k) = \sum_{n=t}^{N} N_n p_n^{(t)}(s_k) - \sum_{m=1}^{t} \sum_{d=m}^{D} \binom{t}{m} H^{(t-m)}(s_k) D_d p_d^{(m)}(s_k) \tag{12}$$

If $p_n^{(t)}$ is the t^{th} order derivative of the n^{th} order numerator polynomial, $p_d^{(t)}$ is the t^{th} order derivative of the d^{th} order denominator polynomial, and $H^{(t)}$ is the t^{th} order derivative of the frequency domain data. All derivatives are relative to $j2\pi f$.

The set of equations at all frequencies s_k and for all derivatives t, can be solved in terms of the unknowns N_n and D_d.

To avoid a breakdown of the orthonormality, virtual samples are introduced when frequency derivatives are included.

2.4 Optimality Polynomial Basisfunctions

Although the orthonormal basis, as used in (6) or (10), provides an improvement in conditioning compared to solving a Vandermonde matrix, the choice of the basis functions is not always optimal.

In fact, better results can be obtained when the numerator and denominator expression is expanded in a different basis of orthonormal polynomials [8]. Suppose the orthonormality is defined with respect to the following inner product.

$$\sum_{\forall k} w_k p_i(s_k)(w_k p_j(s_k))^* = \delta_{ij} \quad \forall 0 \le i,j < K \tag{13}$$

For the numerator polynomials, the weighting function w_k is defined as 1, and for the denominator polynomials, the weighting function is defined as $H(s_k)$. After orthonormalising the numerator and denominator polynomials separately, the matrices Q^{num} and Q^{den} can be calculated. Then the normal equations are given by

$$A^T A \begin{pmatrix} N \\ D \end{pmatrix} = A^T b \tag{14}$$

with $A = \left(Q^{num}{}_{0:N} \quad -HQ^{den}{}_{1:D}\right)$, and $b = \left(HQ^{den}{}_0\right)$ [9]. Due to the orthonormality, $A^T A$ is structured in the following way

$$A^T A = \begin{pmatrix} I_N & X \\ X^T & I_D \end{pmatrix} \tag{15}$$

provided that $X = -\Re e((Q^{num^*}{}_{0:N})^T (Q^{den}{}_{1:D}))$, and $A^T b$ is given as

$$A^T b = \begin{pmatrix} \Re e((Q^{num^*}{}_{0:N})^T Q^{den}{}_0) \\ 0 \end{pmatrix} \tag{16}$$

In [10], it was proved that this polynomial basis is optimal, in a sense that no other polynomial basis can be found resulting in a better conditioned form of the normal equations. Note however, that the structure of these matrices is lost when frequency derivatives are taken into account.

For more information about the calculation of the basis functions, the reader is referred to [9][6][11]. The inclusion of frequency derivatives in combination with adaptive sampling [12] is described in [6].

3. EXAMPLE

The transmission-line coefficient S_{12} of a 2-port Lowpass Filter is modeled over the frequency range [2 GHz – 6 GHz]. All data samples are simulated with the planar full-wave electro-magnetic simulator Agilent EEsof Momentum [13].

15 data samples are selected, which are equidistantly spaced over the frequency range of interest, and a rational approximant is calculated using the technique as described in §2.2. The fitting model is calculated without making use of any frequency derivatives.

Figure 1 shows the rational fitting model (dotted line), and compares it to very densely sampled reference data (full line) on the left axis. The fitting error is shown on the right axis, as a dashed line.

Clearly, the fitting model has an accuracy of approximately –15.3779 dB, which is definitely not sufficient. Now, suppose that the first order frequency derivatives can be obtained from the simulator.

Figure 2 shows the calculated fitting model, based on the same 15 data samples, however in this example, the first order frequency derivatives are taken into account. The additional information can be exploited by the algorithm, and now the fitting model has an accuracy of approximately –70.6604 dB, which is quite accurate. Note that the magnitude of the fitting model closely matches the shape of the reference data.

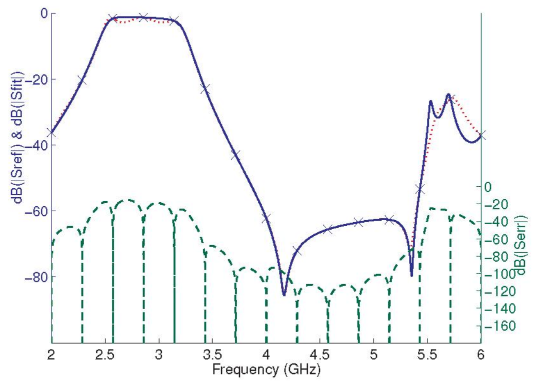

Fig 1 : Rational modeling of Lowpass Filter, based on 15 data samples. Magnitude of rational model (dotted line), and reference data (full line) shown on left axis. Fitting error (dashed line) shown on right axis. No frequency derivatives used.

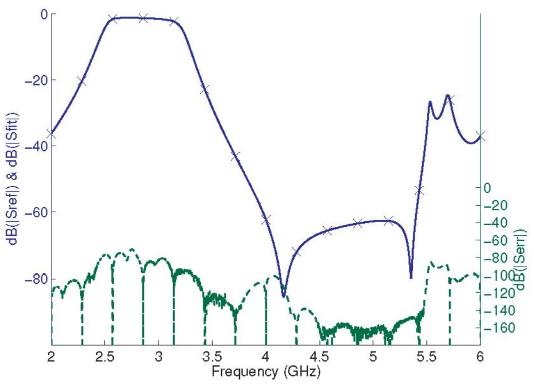

Fig 2 : Rational modeling of Lowpass Filter, based on 15 data samples and first order derivatives. Magnitude of rational model (dotted line), and reference data (full line) shown on left axis. Fitting error (dashed line) shown on right axis. First order frequency derivatives used.

4. CONCLUSIONS

In this paper, a rational least-squares technique is described, which includes frequency derivatives in the modeling process. Orthonormal polynomials are used to improve the numerical accuracy of the approximation problem. Some considerations are given about the optimal choice of polynomial basis functions.

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