Rational Modeling of Spectral Data using Orthonormal Vector Fitting

D. Deschrijver and T. Dhaene
Computational Modeling and Programming (CoMP)
Middelheimlaan 1, 2020 Antwerp, Belgium
dirk.deschrijver@ua.ac.be, tom.dhaene@ua.ac.be

Abstract

Vector Fitting (VF) is an iterative rational macromodeling technique [1] that became quite popular over the last years, due to its simplicity and availability. Although the VF method provides accurate broadband macromodels, the numerical stability of the algorithm is not always optimal. In this paper, the Orthonormal Vector Fitting (OVF) algorithm is introduced, which reduces the numerical sensitivity of the model parameterization to the choice of starting poles significantly, and limits the number of required iterations.

Introduction

Compact rational macromodels, based on measurements or simulations, are very important for efficient time domain and frequency domain simulation of high-speed interconnection structures.

Traditionally, a Vandermonde-like system of equations needs to be solved, in order to determine the system parameters of the rational macromodel. This approach, based on power series is quite straightforward, but its accuracy is limited. The use of alternative polynomial bases, e.g. orthogonal Chebyshev polynomials of the first kind [4], is well-described in literature, but this approach doesn't resolve all numerical issues.

Quite recently in 1999, an iterative least-squares approach (called Vector Fitting) [1], was proposed by Gustavsen and Semlyen, which is essentially a reformulation of the Sanathanan-Koerner iteration [2] with rational basis functions. A detailed analysis and a more general framework of the iterative behaviour and convergence properties of the algorithm is discussed in [3]. This paper, will focus on improvements of the numerical stability and robustness of the VF algorithm. It will be shown that several numerical aspects of Vector Fitting can be improved when orthonormal rational functions are used. This reduces the numerical sensitivity of the model parameterization to the choice of the (starting) poles significantly, and can provide accurate macromodels in fewer iterations.

1 Rational approximation of data

A Linear Time-Invariant (LTI) system can be characterized in the frequency domain by fitting the spectral data to a rational macromodel in a least squares sense.

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

The approximation model is usually built by minimizing the linearized cost function E in terms of the unknown system variables N_n and D_d.

$$E = \sum_{k=0}^{K} \left| \sum_{d=0}^{D} D_d s_k^d f(s_k) - \sum_{n=0}^{N} N_n s_k^n \right|^2 \tag{2}$$

Unfortunately the normal equations of this least-squares problem are often ill-conditioned, especially for highly dynamic systems which cover a large frequency range or require a lot of poles.

A solution to this problem was proposed by Adcock and Potter in 1985 [4]. Instead of expanding the rational basis functions in the power series basis, the equations are much better conditioned when the numerator and denominator are expanded in a basis of orthogonal Chebyshev polynomials of the first kind. The large variations of the Chebyshev polynomials make it possible to downsize the effects of the ill-conditioned matrix, by summing the orthogonal Chebyshev polynomials, instead of summing the power series, which show little variation with increase in order. Unfortunately, although the parameterization becomes much less sensitive to rounding errors, it is much harder to determine the poles and the zeros of the rational model in an accurate way.

However, one could also use rational basis functions, say $\varphi(s)$, instead of polynomial bases.

$$R(s) = \frac{N(s)}{D(s)} = \frac{N_0 + \sum_{n=1}^{N} N_n \varphi_n(s)}{D_0 + \sum_{d=1}^{D} D_d \varphi_d(s)} \tag{3}$$

In order to obtain a proper rational function $R(s)$, the rational basis functions must span the space $\mathcal{L}_n$ which is defined as

$$\mathcal{L}_n = span\{\varphi_0(s), ..., \varphi_P(s)\} \tag{4}$$

$$= \left\{ \frac{p_n(s)}{\pi_n(s)} : p_n \in \Pi_n,\ \pi_n(s) = \prod_{p=1}^{P} (s + a_p) \right\} \tag{5}$$

where Π_n denotes the space of polynomials of degree equal to or less than n. $-a_p$ are chosen to be the poles of the rational basis functions, and $\varphi_0(s)$ is assumed to be a constant e.g. 1. Since $R(s)$ represents a ratio of two rational functions (3), of which the poles of both the numerator and denominator expression contain the (same) roots of $\pi_n(s)$, they are cancelled out when the formulation is simplified and a representation as in (1) is obtained. This approach has several numerical advantages as will be shown further on. First, let's focus on the identification of the system variables. The major difficulty with least-squares rational approximation is that the problem is still non-linear in terms of N_n and D_d. One option, which is commonplace in the engineering world, is to linearize the problem by multiplying left hand side and right hand side of (3) with the denominator expression. Hence, the following set of equations is obtained ($D_0 = 1$)

$$\sum_{n=0}^{N} N_n \varphi_n(s) - R(s) \left(\sum_{d=1}^{D} D_d \varphi_d(s) \right) = R(s) \tag{6}$$

Note that this system of equations (evaluated at all discrete frequencies s) is no longer Vandermonde-like if the $\varphi(s)$ are rational. In fact, when these basis functions are chosen carefully, the model parameterization is significantly better conditioned. This will become clear when we compare this "linearized least-squares" formulation to the Vector Fitting technique in the next paragraph.

2 Vector Fitting technique

The Vector Fitting technique approximates the frequency response with a rational pole-residue model $R(s)$.

$$R(s) = \sum_{p=1}^{P} \frac{c_p}{s + a_p} + c_0 \tag{7}$$

$R(s)$ approximates the simulated data samples at the discrete complex frequencies s. $-a_p$ and c_p are the poles and residues respectively, $\forall p = 1, ..., P$ and c_0 is a constant. The "weighted" data is approximated by a rational function $\bar{R}(s)$ based on an initial set of starting poles $-\bar{a}_p$

$$\bar{R}(s) = \sum_{p=1}^{P} \frac{c_p}{s + \bar{a}_p} + c_0 \tag{8}$$

This rational function approximates equation (7) multiplied by an unknown rational "weighting" function $\sigma(s)$. Since $\sigma(s)$ is also rational, it can be represented in pole-residue form, which leads to the following augmented problem

$$\begin{bmatrix} \sigma(s)R(s) \\ \sigma(s) \end{bmatrix} = \begin{bmatrix} \sum_{p=1}^{P} \frac{c_p}{s+\bar{a}_p} + c_0 \\ \sum_{p=1}^{P} \frac{\tilde{c}_p}{s+\bar{a}_p} + 1 \end{bmatrix} \tag{9}$$

The augmented problem can be linearized in terms of the unknowns c_p, d, h and $\tilde{c}_p$ by multiplying the second line of the vector equation with $R(s)$.

$$\left(\sum_{p=1}^{P} \frac{c_p}{s + \bar{a}_p} + c_0 \right) = \left(\sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \bar{a}_p} + 1 \right) R(s) \tag{10}$$

or

$$(\sigma R)_{fit}(s) = \sigma_{fit}(s) R(s) \tag{11}$$

Hence, the following set of linear equations is obtained

$$\sum_{p=1}^{P} \frac{c_p}{s + \bar{a}_p} + c_0 - R(s) \left(\sum_{p=1}^{P} \frac{\tilde{c}_p}{s + \bar{a}_p} \right) = R(s) \tag{12}$$

Remark that this form reduces exactly to (6)

$$\sum_{p=0}^{P} c_p \varphi_p(s) - R(s) \left(\sum_{p=1}^{P} \tilde{c}_p \varphi_p(s) \right) = R(s) \tag{13}$$

when the $\varphi_p(s)$ are chosen to be the basis functions of the partial fraction expansion of a rational function.

$$\varphi_0(s) = 1, \varphi_p(s) = \frac{1}{s + \bar{a}_p} \tag{14}$$

Once the unknown parameters are estimated, $R(s)$ can easily be obtained as

$$R(s) = \frac{\sum_{p=0}^{P} c_p \varphi_p(s)}{\sum_{p=0}^{P} \tilde{c}_p \varphi_p(s)} \tag{15}$$

Similarly, this ratio of rational functions with common denominator reduces after simplification to the classical pole-residue form (7) or the ratio of polynomials (3). The main conclusion of this paragraph is that the so-called "pole identification" of Vector Fitting reduces exactly to an iterative version of the "linearized least squares" formulation in the previous paragraph.

Note that the basis functions, chosen in the Vector Fitting technique, are the classical partial fraction expansion of a rational model. These basis functions are mainly responsible for the conditioning of the Vector Fitting technique, since they occur directly in the equations that need to be solved. In the next paragraph, it will be shown that alternative basis functions can be used as well.

3 The use of alternative basis functions

Instead of using the partial fractions as rational basis functions, it will be shown that orthonormal rational basis functions can lead to significant improvements in numerical conditioning [5]. A straightforward way to calculate an orthonormal basis, is to apply a Gram-Schmidt procedure on the partial fractions [6][7]. Hence, orthonormal rational functions $\phi_p(s)$ are obtained, which are in fact linear combinations of the partial fractions $\varphi_p(s)$, of the form

$$\phi_p(s) = \frac{Q_p(s)}{\prod_{j=1}^{p}(s + a_j)} \tag{16}$$

for $p = 1, ..., P$ and $Q_p(s)$ an arbitrary polynomial of order $p - 1$.

$$\langle \phi_i(s), \phi_j(s) \rangle = \delta_{ij} \tag{17}$$

The inner product is defined as

$$\langle \phi_i(s), \phi_j(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_i(s) \phi_j^*(s) ds \tag{18}$$

As an example, consider the construction of the first function $\phi_1(s)$.

$$\langle \phi_1(s), \phi_1(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_1(s) \phi_1^*(s) ds \tag{19}$$

$$= \frac{1}{2\pi i} \int_{i\mathbb{R}} \frac{|\gamma_1|^2}{(s + a_1)(-s + a_1^*)} ds \tag{20}$$

$$= \frac{|\gamma_1|^2}{a_1 + a_1^*} \tag{21}$$

To normalize $\phi_1(s)$, $Q_1(s) = \gamma_1$ must equal $\kappa_1 \sqrt{2\Re e(a_1)}$, where κ_1 is an arbitrary unimodular complex number. $\phi_1(s)$ is then obtained as

$$\phi_1(s) = \kappa_1 \sqrt{2\Re e(a_1)} \frac{1}{s + a_1} \tag{22}$$

Now consider the construction of the second function $\phi_2(s)$. First of all, $\phi_2(s)$ must be orthogonal to $\phi_1(s)$

$$\langle \phi_1(s), \phi_2(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_1(s) \phi_2^*(s) ds = 0 \qquad (23)$$

which implies that $\phi_2^*(s)$ must vanish for $s = -a_1$. Therefore $Q_2(s) = \gamma_2(s - a_1^*)$. This constant γ_2 is determined by imposing the normalization condition

$$\begin{aligned} & \langle \phi_2(s), \phi_2(s) \rangle \\ = & \frac{1}{2\pi i} \int_{i\mathbb{R}} \frac{\gamma_2(s-a_1^*)}{(s+a_1)(s+a_2)} \frac{\gamma_2^*(-s-a_1)}{(-s+a_1^*)(-s+a_2^*)} ds \qquad (24) \\ = & \frac{1}{2\pi i} \int_{i\mathbb{R}} \frac{|\gamma_2|^2}{(s+a_2)(-s+a_2^*)} ds = \frac{|\gamma_2|^2}{a_2 + a_2^*} \qquad (25) \end{aligned}$$

Clearly, it follows that $\gamma_2 = \kappa_2 \sqrt{2\Re e(a_2)}$, where κ_2 is an arbitrary unimodular complex number. So, $\phi_2(s)$ is then given by

$$\phi_2(s) = \kappa_2 \sqrt{2\Re e(a_2)} \frac{s - a_1^*}{(s+a_1)(s+a_2)} \qquad (26)$$

Similarly continuing this approach, the general polynomials are obtained

$$\phi_p(s) = \kappa_p \left(\prod_{j=1}^{p-1} \frac{s - a_j^*}{s + a_j} \right) \sqrt{2\Re e(a_p)} \frac{1}{s + a_p} \qquad (27)$$

The calculation of this basis is not new, but is given here for the sake of completeness and ease of understanding. In fact, orthogonal rational functions have a long history in mathematics and engineering. This basis originates from the discrete-time Takenaka-Malmquist basis [8]-[9], originally developped in 1925, and has later been transformed to the continuous time domain. It is a generalization of the Laguerre basis [10], where all poles $\{-a_p\}$ are the same real number, and the Kautz bases [11] where all poles $\{-a_p, -a_{p+1}\}$ are the same complex conjugate pair with $-a_p^* = -a_{p+1}$.

For the macromodeling of LTI systems, the basis functions must have real coefficients, hence a linear combination of $\phi_i(s)$ and $\phi_{i+1}(s)$ is formed

$$\begin{aligned} & \alpha\phi_i(s) + \beta\phi_{i+1}(s) \\ = & \left(\prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{\alpha(s + a_{i+1}) + \beta(s - a_i^*)}{(s + a_i)(s + a_{i+1})} \qquad (28) \\ = & \left(\prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{s(\alpha + \beta) + (\alpha a_{i+1} - \beta a_i^*)}{(s + a_i)(s + a_{i+1})} \qquad (29) \end{aligned}$$

which can be made real-valued if $a_{i+1} = a_i^*$ (or if both a_i and a_{i+1} are real). This way, two orthonormal functions of the following form are obtained

$$\phi_i(s) = \gamma_i \left(\prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{s - x}{(s + a_i)(s + a_{i+1})} \qquad (30)$$

$$\phi_{i+1}(s) = \gamma_{i+1} \left(\prod_{j=1}^{i-1} \frac{s - a_j^*}{s + a_j} \right) \frac{s - y}{(s + a_i)(s + a_{i+1})} \qquad (31)$$

with real $\gamma_i, \gamma_{i+1}, x$ and y. To impose the orthogonality,

$$\langle \phi_i(s), \phi_{i+1}(s) \rangle = \gamma_i \gamma_{i+1} \frac{xy + a_i a_{i+1}}{2(a_i + a_{i+1}) a_i a_{i+1}} = 0 \qquad (32)$$

x and y are set to be $\sqrt{a_i a_{i+1}}$ and $-\sqrt{a_i a_{i+1}}$ respectively. Similarly, γ_i and γ_{i+1} are set to $\sqrt{a_i + a_{i+1}}$. Note that this choice is not unique, and that other possibilities exist.

Implementing these orthonormal rational basis functions in VF (see Section II and III) leads to OVF. The OVF technique makes the model parameterization significantly better conditioned, especially if the poles are real, or the magnitude of the real part of the complex poles is non-negligible. Unstable poles can either be flipped into the left half plane or deleted in each iteration. Passivity can be enforced as post-processing technique [13][14][15].

4 Example

The reflection coefficient S_{11} of a Quarter Wavelength Filter (QWVL) is modeled over the frequency range of interest [1 GHz - 12 GHz], based on a set of 32 equidistant support samples. The initial poles are chosen as complex conjugate pairs (imaginary parts equidistantly spread over the frequency range of interest), with a fixed real part. Both techniques (VF and OVF) are used to fit the rational data using the same set of initial poles, and are allowed one single iteration. Table 1 shows the condition number of both techniques (ratio between largest and smallest singular value) when the real part of the poles varies from -1 to -5. Clearly, the new technique is significantly better conditioned when the distance between the poles and the imaginary axis increases. Fig. 1 shows both rational fits, and their corresponding error when the real part is set to -5. Fig. 2 shows the corresponding singular values of the "pole identification". Due to numerical problems, VF was unable to provide accurate results in only 1 iteration. Using OVF, on the other hand, numerical problems are avoided and the accuracy is almost twice as good. In general, the best results for both techniques are obtained when the initial poles are chosen as described in [1].

5 Conclusion

In this paper, the Vector Fitting technique is modified such that orthonormal rational functions are used during the fitting process. Several examples show that this approach improves the numerical conditioning of the pole-identification significantly. The Orthonormal Vector Fitting (OVF) technique can provide accurate results when the starting poles are not chosen optimally, often in fewer iterations.

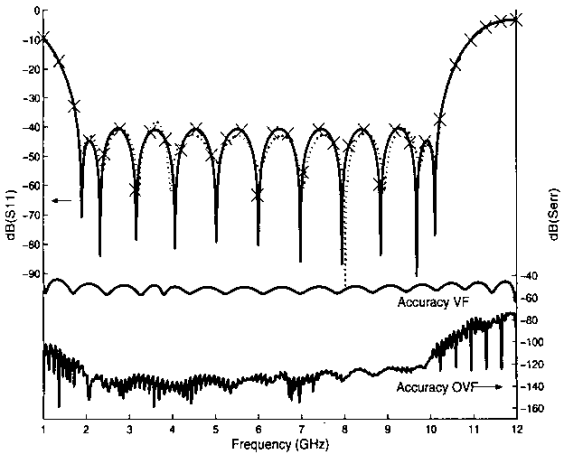

Figure 1: Left : Magnitude S_{11} of QWVL using VF (dashed) and OVF (full). Right : Accuracy of the fit

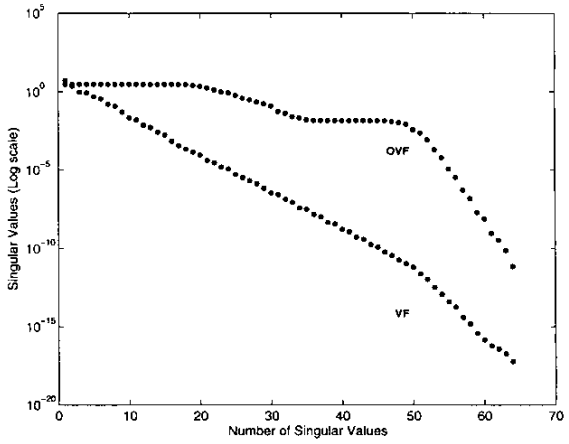

Figure 2: Singular Values of QWVL (VF and OVF).

$\Re e(-a_p)$	Cond.Nr. VF	Cond.Nr. OVF
-5	8.5856×10^{17}	4.2810×10^{11}
-4	5.4016×10^{16}	2.3412×10^{10}
-3	1.9729×10^{14}	1.0428×10^{9}
-2	3.6305×10^{11}	5.6707×10^{7}
-1	4.6070×10^{8}	4.9655×10^{7}

Table 1: Conditioning vs. pole location.

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References

[1] Gustavsen, B., Semlyen, A., "Rational Approximation of Frequency Domain Responses by Vector Fitting", *IEEE Trans. of Power Delivery*, Vol. 14 (1999), pp. 1052-1061.

[2] Sanathanan, C., Koerner, J., "Transfer Function Synthesis as a Ratio of two Complex Polynomials", *IEEE Trans. on Automatic Control*, Vol. 8, No. 1 (1963), pp. 56-58.

[3] Hendrickx, W., Deschrijver, D., Dhaene, T., "Some Remarks on the Vector Fitting Iteration", *Submitted to Lecture Notes on Computer Science.*

[4] Adcock, J., Potter, R., "A Frequency Domain Curve Fitting Algorithm with Improved Accuracy", *Proc. 3rd International Model Analysis Conference*, Vol. 1 (1985), pp. 541-547.

[5] Ninness, B., Gibson, S., Weller, S.R., "Practical Aspects of using Orthonormal System Parameterisations in Estimation Problems", *12th IFAC Symposium on System Identification* (2002).

[6] Akcay, H., Ninness, B., "Orthonormal Basis Functions for Modelling Continuous-Time Systems," *Signal Processing*, Vol. 77, No. 1 (1999), pp. 261-274.

[7] Oliveira e Silva, T., "Rational Orthonormal Functions on the Unit Circle and on the Imaginary Axis, with Applications in System Identification" (1995).

[8] Takenaka, S., "On the Orthogonal Functions and a New Formula of Interpolation", *Japanese Journal of Mathematics*, (1925), pp. 129-145.

[9] Malmquist, F., "Sur la détermination d'une classe de fonctions analytiques pas leurs valeurs dans un ensemble donné de points", *Compte Rendus de Sixieme Congres des Mathematiciens Scandinaves*, (1926), pp. 253-259.

[10] Clement, P.R., "Laguerre Functions in Signal Analysis and Parameter Identification", *Journal of the Franklin Institure*, Vol. 313, (1982), pp. 85-95.

[11] Kautz, W.H., "Transient Synthesis in the Time-Dómain", *IRE Trans. on Circuit Theory*, Vol. 1 (1954), pp. 29-39.

[12] Szabo, Z., Heuberger, P.S.C, Bokor, J., Van Den Hof, P.M.J, "Extended Ho-Kalman Algorithm for Systems Represented in Generalized Orthonormal Bases", *Automatica*, Vol.37, No. 10 (2001), pp. 1593-1600.

[13] Grivet-Talocia, S., "Enforcing Passivity of Macromodels via Spectral Perturbation of Hamiltonian Matrices", *7th IEEE Workshop on Signal Propagation on Interconnects*, (2003), pp. 33-36.

[14] Gustavsen, B., Semlyen, A., "Enforcing Passivity for Admittance Matrices approximated by Rational Functions", *IEEE Trans. on Power Systems*, Vol. 16 (2001), pp. 97-104.

[15] Saraswat, D., Achar, R., Nakhla, M., "A Fast Algorithm and Pratical Considerations For Passive Macromodeling of Measured/Simulated Data", *IEEE Trans. on Comp., Packaging and Manuf. Tech.*, Vol. 27, No. 1 (2004), pp. 57-70.