Macromodeling of transfer functions with higher-order pole multiplicities*

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Abstract

Vector Fitting is a rational approximation technique, which is frequently used to calculate accurate macromodels of electrical and electronical structures [1]. The robustness of the technique is obtained by combining the use of a weighted iterative least squares scheme and a well-chosen partial fraction basis. It was discussed in [2] that numerical problems may occur if poles of higher-order multiplicities are required to approximate a frequency response. This paper shows that the Orthonormal Vector Fitting technique [3] solves this problem in a fundamental way.

1 Introduction

Vector Fitting is a broadband macromodeling technique, which calculates a rational transfer function based on simulation- or measurement based data [1]. The method is essentially a reformulation of the Sanathanan-Koerner iteration [4], provided that the numerator and denominator are jointly expanded in a basis of partial fractions [5]. In the original description of the Vector Fitting technique, it is assumed that the prescribed (or relocated) poles of the basis functions always occur with a single multiplicity.

Recently, it was shown that numerical ill-conditioning can result if some basis functions are based on a pole with higher-order multiplicity [6]. Especially when the normal equations are solved, numerical rank deficiency may already occur if some poles are located arbitrarily close. In order to overcome these difficulties, an extension of the basis functions was presented to overcome this problem [3]. Even though the extension can enhance the fitting accuracy, it requires a clustering of poles before each pole-relocation in order to improve numerical conditioning [7]. The clustering requires an additional computational cost, and is not always trivial since it partially relies on heuristics.

In this paper, it is shown that the Orthonormal Vector Fitting (OVF) algorithm [8] tackles the problem in a more fundamental way. Several examples show that the proposed approach is robust and leads to a better overall result.

2 Identification Technique

The goal of the Vector Fitting technique, is to approximate the frequency domain data samples $\{(s_k, H(s_k)\}_{k=0}^{K}$ by a rational function $R(s)$. To obtain a robust procedure, the numerator and denominator of the transfer function are expanded as a linear combination of partial fractions which are based on a prescribed set of stable poles $a = \{-a_p\}_{p=1}^{P}$. These poles are chosen to be real or occur as complex conjugate pairs, such that $a = \{-a_{p,r}\}_{p=1}^{P_r} \cup \{-a_{p,c}, -a_{p,c}^*\}_{p=1}^{P_c}$.

In successive iterations, the VF technique relocates these poles towards more optimal locations by solving the pole-identification equations (1) and an eigenvalue problem as described in [1]. If some of the poles occur with a higher-order multiplicity, then the partial fraction basis functions become linearly dependent. This results that the system equations associated with cost function (1) become singular, or close to singular if the basis function poles are located arbitrarily close.

In [3], an extension of the basis functions and a generalized state-space realization is proposed (VFe) [9]. Assume that the set of P_r (P_c) real (complex pairs of) poles consists of M_r (M_c) distinct poles having multiplicity $v_{p,r}$ ($v_{p,c}$), then a generalized expression of the cost function can be formulated as in (2). Using these extended basis functions, it was shown that numerical ill-conditioning can be avoided if "close poles" (which may occur during the iterations of the algorithm) are clustered before each pole-relocation. In practice, it is not a trivial task to decide if a set of "close poles" really corresponds to a pole with higher-order multiplicity, and to pinpoint the optimal center of such a cluster.

3 Orthonormal Vector Fitting

This paper proposes the use of Orthonormal Vector Fitting to resolve the issues in a robust way. Rather than using the partial fraction expansion of a rational function, a set of orthonormal rational functions $\phi_p(s)$ is chosen, which are defined as

$$\phi_{p,r}(s_k) = \frac{\sqrt{2\Re e(a_p)}}{s_k + a_p} \left(\prod_{j=1}^{p-1} \frac{s_k - a_j^*}{s_k + a_j} \right) \quad (4)$$

if the pole $-a_p$ is real, and

$$\phi_{p,c}(s_k) = \frac{\sqrt{2\Re e(a_p)}(s_k - |a_p|)}{(s_k + a_p)(s_k + a_{p+1})} \left(\prod_{j=1}^{p-1} \frac{s_k - a_j^*}{s_k + a_j} \right) \quad (5)$$

$$\phi_{p+1,c}(s_k) = \frac{\sqrt{2\Re e(a_p)}(s_k + |a_p|)}{(s_k + a_p)(s_k + a_{p+1})} \left(\prod_{j=1}^{p-1} \frac{s_k - a_j^*}{s_k + a_j} \right) \quad (6)$$

if $-a_p = -a_{p+1}^*$ form a complex conjugate pair of poles. This set of functions is obtained by a Gram-Schmidt orthonormalization [10] on the set of partial fractions, with respect to the following continuous inner product ($1 \leq m, n \leq P$) [11].

$$\langle \phi_m(s), \phi_n(s) \rangle = \frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_m(s) \phi_n^*(s) ds \quad (7)$$

Theorem 3.1 shows that the orthonormal basis functions do not become linearly dependent if some of the poles occur with a higher-order multiplicity, provided that they are located in the closed left half plane ($\Re e(-a_p) < 0$).

*This work was supported by the Fund for Scientific Research Flanders (FWO Vlaanderen)

$$\arg\min_{c_p,\tilde{c}_p} \left(\sum_{k=0}^{K} \left| \left(\sum_{p=1}^{P_r} \frac{c_{p,r}}{s_k + a_{p,r}} + \sum_{p=1}^{P_c} \left(\frac{c_{p,c}}{s_k + a_{p,c}} + \frac{c_{p,c}^*}{s_k + a_{p,c}^*} \right) \right) \right.\right.$$
$$\left.\left. -H(s_k) \left(1 + \sum_{p=1}^{P_r} \frac{\tilde{c}_{p,r}}{s_k + a_{p,r}} + \sum_{p=1}^{P_c} \left(\frac{\tilde{c}_{p,c}}{s_k + a_{p,c}} + \frac{\tilde{c}_{p,c}^*}{s_k + a_{p,c}^*} \right) \right) \right|^2 \right) \quad (1)$$

$$\arg\min_{c_{pm},\tilde{c}_{pm}} \left(\sum_{k=0}^{K} \left| \left(\sum_{p=1}^{M_r} \sum_{m=1}^{v_{p,r}} \frac{c_{pm,r}}{(s_k + a_{p,r})^m} + \sum_{p=1}^{M_c} \sum_{m=1}^{v_{p,c}} \left(\frac{c_{pm,c}}{(s_k + a_{p,c})^m} + \frac{c_{pm,c}^*}{(s_k + a_{p,c}^*)^m} \right) \right) \right.\right.$$
$$\left.\left. -H(s_k) \left(1 + \sum_{p=1}^{M_r} \sum_{m=1}^{v_{p,r}} \frac{\tilde{c}_{pm,r}}{(s_k + a_{p,r})^m} + \sum_{p=1}^{M_c} \sum_{m=1}^{v_{p,c}} \left(\frac{\tilde{c}_{pm,c}}{(s_k + a_{p,c})^m} + \frac{\tilde{c}_{pm,c}^*}{(s_k + a_{p,c}^*)^m} \right) \right) \right|^2 \right) \quad (2)$$

$$\arg\min_{c_p,\tilde{c}_p} \left(\sum_{k=0}^{K} \left| \left(\sum_{p=1}^{P_r} c_{p,r}\phi_{p,r}(s_k,a) + \sum_{p=1}^{P_c} \left(c_{p,c}\phi_{p,c}(s_k,a) + c_{p,c}^*\phi_{p+1,c}(s_k,a) \right) \right) \right.\right.$$
$$\left.\left. -H(s_k) \left(1 + \sum_{p=1}^{P_r} \tilde{c}_{p,r}\phi_{p,r}(s_k,a) + \sum_{p=1}^{P_c} \left(\tilde{c}_{p,c}\phi_{p,c}(s_k,a) + \tilde{c}_{p,c}^*\phi_{p+1,c}(s_k,a) \right) \right) \right|^2 \right) \quad (3)$$

Theorem 3.1 *The orthonormal rational basis functions $\{\phi_p(s)\}_{p=1}^{P}$ are linearly independent if they are based on stable poles with a non-zero real part ($\phi_p(s) \neq 0$).*

Proof The proof of this theorem is given by contradiction (*reductio ad absurdum*). Assume that the functions $\{\phi_p(s)\}_{p=1}^{P}$ are not linearly independent. This means that some basis function $\phi_p(s)$ can be expanded as a linear combination of the other basis functions

$$\phi_p(s) = \sum_{j=1, j\neq p}^{P} \alpha_j \phi_j(s) \quad (8)$$

Therefore, it follows that

$$\langle \phi_p(s), \phi_p(s) \rangle = \left\langle \phi_p(s), \sum_{j=1,j\neq p}^{P} \alpha_j \phi_j(s) \right\rangle \quad (9)$$
$$= \frac{1}{2\pi i} \int_{i\mathbb{R}} \sum_{j=1,j\neq p}^{P} \alpha_j \phi_j(s) \phi_p^*(s) ds \quad (10)$$
$$= \sum_{j=1,j\neq p}^{P} \alpha_j \left(\frac{1}{2\pi i} \int_{i\mathbb{R}} \phi_j(s) \phi_p^*(s) ds \right) \quad (11)$$
$$= 0 \quad (12)$$

This contradicts the fact that the basis functions are orthonormal, i.e. $\langle \phi_p(s), \phi_p(s) \rangle = 1$, hence the initial assumption that the basis functions are linearly dependent is false. ⊡

It follows from this theorem that poles of higher-order multiplicity will not result in linearly dependent columns of the system equations (i.e. rank deficiency), provided that the orthonormal basis functions are used instead of partial fractions. Therefore, it is preferable to minimize cost function (3).

4 Example : RLC Filter

The following highly dynamical frequency response of an RLC filter of order 18 is considered over the frequency range [1 Hz - 100 KHz], as shown in Figure 1.

$$H(s) = \frac{40 + 60000i}{(s + 220 + 45000i)^3} + \frac{40 - 60000i}{(s + 220 - 45000i)^3} + \frac{-150 + 40000i}{(s + 220 + 20000i)^3} + \frac{-150 - 40000i}{(s + 220 - 20000i)^3} + \frac{-5 + 7000i}{(s + 220 + 5000i)^3} + \frac{-5 - 7000i}{(s + 220 - 5000i)^3} \quad (13)$$

The response contains 3 distinct pairs of complex conjugate poles, each with a higher-order multiplicity of 3.

A rational fitting model is constructed using Vector Fitting (VF), Vector Fitting with extended basis functions (VFe), and the Orthonormal Vector Fitting (OVF). In all examples, the initial poles are "optimally chosen" [1] as complex conjugate pairs with small real parts, and with imaginary parts equidistantly spread over the frequency range of interest. Three realistic situation are considered where poles and residues are both calculated using QR decomposition (QR/QR), or normal equations (NE/NE) respectively, as well as the hybrid case (NE/QR).

4.1 NE/QR Figure 2 shows the results if the poles are calculated using Normal Equations, and the residues using a QR decomposition (NE/QR). In successive iterations, it is observed that the poles of the VF model are relocated towards the correct locations. However, once the correct poles are reasonably well approximated, the system equations of the next pole-identification step become severely ill-conditioned. The inaccurate relocation of poles in the following iteration causes a reoccuring relapse in the convergence process. This effect is clearly

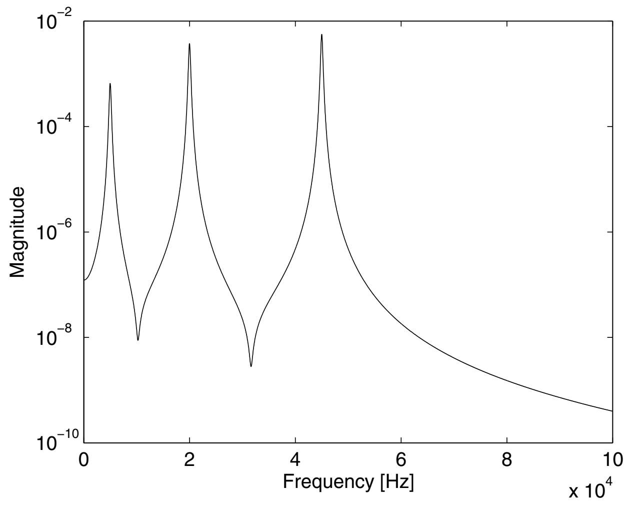

Figure 1: Magnitude of Frequency Response

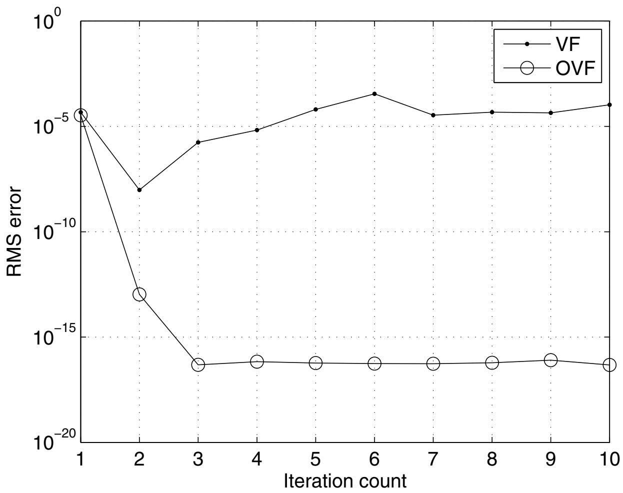

Figure 3: Rational Fitting using NE/NE

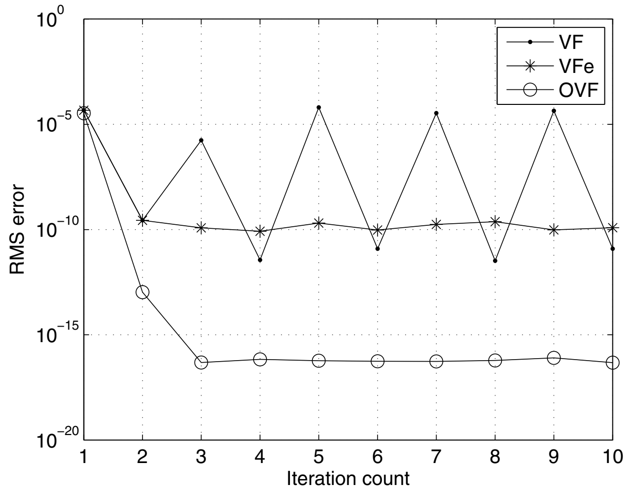

Figure 2: Rational Fitting using NE/QR

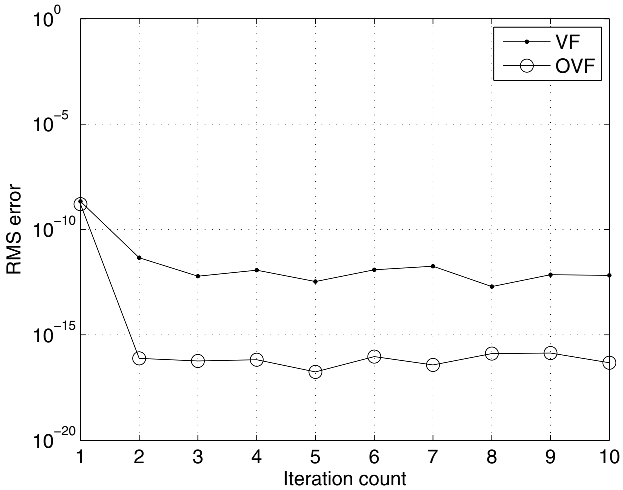

Figure 4: Rational Fitting using QR/QR

illustrated by an oscillating error function.

Using the Vector Fitting approach with extended basis functions (VFe), the evolution of the error function becomes more reliable. However, it is noted that the VFe approach requires a (manual) clustering of poles which are arbitrarily close before each pole-relocation, to avoid numerical problems.

The OVF approach tackles the rank-deficiency at a more fundamental level, and leads to better overall results. It is seen that the fitting error of the rational model is close to machine precision in only 3 iterations. At the same time, it is observed that the VF and VFe technique do not lead to comparable results if additional iterations are performed.

4.2 NE/NE Figure 3 shows that the VF results are rather poor over all iterations if the poles and residues are both solved using Normal Equations (NE/NE). If the pole-identification is ill-conditioned, due to the occurrence of poles with higher-order multiplicity, then it is obvious that a poor fitting model will result [3]. However if the pole-identification is well-conditioned (e.g. in the first iteration where the initial starting poles are chosen to be distinct) then the poles will be identified accurately. The accurate identification of poles means that the residue identification will become ill-conditioned, since it is based on poles of higher-order multiplicity. Therefore, a poor fitting model results during all iterations of the algorithm. If the OVF approach is used, then reliable results are obtained throughout the iterations. Again, the accuracy of the OVF fitting model is close to machine precision in only 3 iterations.

4.3 QR/QR Figure 4 shows the results which are obtained during standard application of the Vector Fitting routine, using QR decomposition for the calculation of poles and residues (QR/QR). It is observed that the RMS error of the VF approximation model is acceptable, but it still does not match the performance of OVF. Clearly, the use of a QR decomposition leads to accurate results in only 2 iterations, and is therefore preferable over the use of Normal Equations, in terms of numerical robustness.

4.4 Identification using correct poles Now, assume that the exact location of the transfer function poles is known in advance. Based on this prior knowledge, only the residue of each basis function needs to be calculated.

Figure 5 shows that the quality of the VF fitting model (dashed) remains unacceptable, even though the poles of the basis functions are exactly known. It is also observed that there is no visible difference between the data (solid line), and the model which is calculated using the VFe or OVF technique (dotted line).

As shown in Table I, the corresponding RMS errors using the VFe and OVF technique are comparable, and very close to machine precision. This result illustrates that the classical VF technique can not be applied if some of the basis functions are based on identical poles, even when a QR decomposition is used as matrix solver.

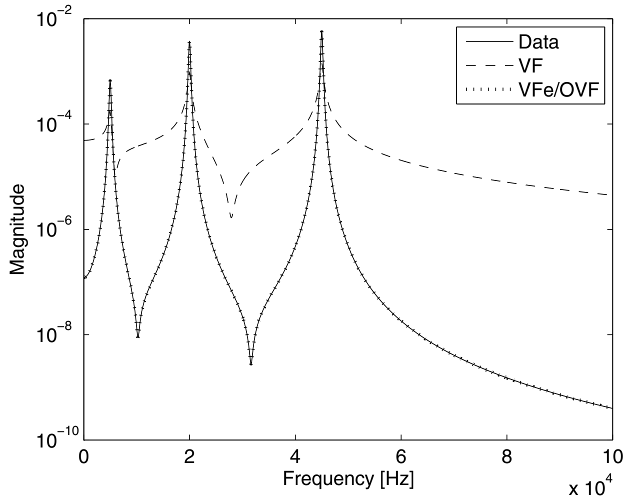

Figure 5: Residue calculation using correct poles

Table 1: RMS Error of Fitting Model

Method	Normal Equations	QR Decomposition
VF	NaN	$3.1608 * 10^{-4}$
VFe	$7.4168 * 10^{-18}$	$1.0031 * 10^{-18}$
OVF	$3.8523 * 10^{-17}$	$3.8542 * 10^{-17}$

5 Conclusions

This paper advocates the use of Orthonormal Vector Fitting for the macromodeling of transfer functions which have poles of higher-order multiplicity. It is shown that more robust results are obtained using OVF, if some poles of the basis functions occur with a higher-order multiplicity during successive iteration steps of the algorithm. This improvement of OVF over previous approaches (VF) is obtained by resolving a fundamental limitation of the partial fraction basis, and is not primarily related to the choice of matrix solver or the initial pole specification. The OVF approach doesn't require a manual clustering of close poles before each relocation, and is therefore preferable over the use of VFe.

6 Acknowledgements

This work was supported by the Fund for Scientific Research, Flanders (FWO-Vlaanderen).

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