# Univariate Rational Macromodeling of High-Speed Passive Components: a Comparative Study

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Accurate broadband macromodels are of paramount importance for the study, design and optimization of RF, microwave, and millimeter-wave components and systems. These compact macromodels approximate the complex electro-magnetic (EM) behavior of high-speed multi-port systems at the input and output ports in the frequency domain by rational functions. It is well-known that the estimation of the system parameters is a numerically ill-conditioned problem. In literature, several techniques are proposed to relieve these numerical issues. This paper gives an overview and comparison of some rational fitting methods, which are most commonly used to model deterministic, simulation based data.

## SECTION 1 INTRODUCTION : MACROMODELING

Compact rational macromodels, based on measurements or full-wave electromagnetic (EM) simulations, are very important for efficient time domain and frequency domain simulation of high-frequency/high-speed interconnections, components and systems. These macromodels characterize the electromagnetic behavior of electrical and electronical components at the input and output ports in the frequency domain (s, H(s)), using rational functions <sup>[24]</sup>.

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n=0}^{N} N_n s^n}{\sum_{d=0}^{D} D_d s^d} \qquad s = j2\pi f \qquad (1.1)$$

The rational model should have a sufficient accuracy  $\delta$  over a predefined frequency range of interest  $[s_0, s_K]$ 

$$dB(|R(s) - H(s)|) < \delta, \ \forall s \in [s_0, s_K]$$

$$(1.2)$$

and it should satisfy several physical properties, which are inherent to linear time-invariant (LTI) systems, such as e.g. causality, system stability and passivity [1, 2].

- (a) The coefficients of the numerator and denominator polynomial must be real, in order to avoid imaginary terms in the time-domain. This implies that the poles and zeros of the rational model are real or occur in complex conjugate pairs (i.e.  $R(s) = R^*(s^*)$ ).
- (b) The order of numerator must be smaller than (or equal to) the order of denominator in the case of scattering parameters. If N > D,

$$\lim_{s \to \infty} \frac{\sum_{n=0}^{N} N_n s^n}{\sum_{d=0}^{D} D_d s^d} = \infty$$
(1.3)

which violates the passivity constraint (e). Also, when considering the partial fraction expansion, the higher order polynomial terms  $s, s^2, \ldots$  would translate to unrealizable derivatives in the time domain.

- (c) To enforce Bounded-Input-Bounded-Output (BIBO) system stability, all poles must be located in the left half of the complex plane. Unstable poles translate to unbounded exponentials in the time domain as s approaches infinity.
- (d) All rational models (in the case of multiport systems) should share a common set of poles, in order to increase the efficiency of the time-domain convolutions.
- (e) If the system is passive (unable to generate energy), the rational model must be passive as well, in order to avoid instabilities in time-domain simulations <sup>[12]</sup>. For scattering parameters, the rational function must be bounded real

$$I - H(s^*)H(s) \ge 0, \ \forall s \tag{1.4}$$

which is equivalent to

$$\max_{i,s}(\sigma_i(s)) \le 1, \ \forall \sigma_i(s) \in \sigma(H(s))$$
(1.5)

where  $\sigma$  represents the singular values, or positive real for hybrid parameters

$$\max_{i,s}(\lambda_i(s)) \ge 0, \ \forall \lambda_i(s) \in \lambda(\Re e(H(s)))$$
(1.6)

where  $\lambda$  represents the eigenvalues. Recall that eigenvalues and singular values of a matrix H are related by

$$\sigma_i \ge 0 \in \sigma(H) \Longleftrightarrow \sigma_i^2 \in \lambda(H^*H) \tag{1.7}$$

Unfortunately, in some cases, 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. Therefore, adaptive techniques <sup>[5, 8]</sup> are used which gradually build up a model by iteratively selecting new samples (and/or frequency derivatives) based on error estimates, while adjusting the model complexity as needed. In this report, the data that is used to characterize these models, is deterministic simulated data (i.e. repeatable and no measurement noise).

In literature, several rational interpolation and rational approximation techniques are proposed to calculate such a rational function. In this report, the most commonly used techniques are selected and compared from a practical point of view. Each approach will be discussed briefly, and some pro's and con's will be given. Afterwards, some numerical results will be given to compare the accuracy and usefullness of all techniques. Matlab code is available at : http://www.coms.ua.ac.be/urm\_toolbox, which should encourage the reader to experiment and get some hands-on experience.

## SECTION 2 RATIONAL MODEL

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

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n=0}^{N} N_n s^n}{\sum_{d=0}^{D} D_d s^d} \qquad \qquad s = j2\pi f \qquad (2.1)$$

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  $(D_0 \text{ can be chosen arbitrarily, e.g. } D_0 = 1)$ , a set of K + 1 = 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 = 0, 1, ..., K. 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.

#### 2.1 Unattainable points

When calculating an interpolant, the problem can easily be linearized by multiplying the left hand side and right hand side of (2.1) with the denominator expression.

$$\sum_{n=0}^{N} N_n s^n = \left(\sum_{d=0}^{D} D_d s^d\right) H(s)$$
(2.2)

While the solution of these homogeneous equations is in general straightforward, the solution of the linearized problem will not always satisfy the rational interpolating conditions (2.1). Moreover, there may even not be a solution to the rational interpolation problem. An interpolating function satisfying (2.1) satisfies (2.2), however the inverse relation doesn't hold in general <sup>[33, 16]</sup>.

**Definition 1** Two rational functions

$$H_1(s) = \frac{N^1(s)}{D^1(s)}, H_2(s) = \frac{N^2(s)}{D^2(s)}$$
(2.3)

are said to be equivalent if

$$N^{1}(s)D^{2}(s) = N^{2}(s)D^{1}(s)$$
(2.4)

Theorem 2 If

$$H_1(s) = \frac{N^1(s)}{D^1(s)}, H_2(s) = \frac{N^2(s)}{D^2(s)}$$
(2.5)

are both non-trivial solutions of the homogeneous linear system (2.2), then they are equivalent.

**Proof.** Let  $X(s) = N^1(s)D^2(s) = N^2(s)D^1(s)$ . Then for k=0,1,...,K

$$X(s_k) = N^1(s_k)D^2(s_k) - N^2(s_k)D^1(s_k)$$
(2.6)

$$= H(s_k)D^1(s_k)D^2(s_k) - H(s_k)D^2(s_k)D^1(s_k)$$
(2.7)

$$= 0$$
 (2.8)

Since the order of X doesn't exceed K-1, X must be identically zero.

This theorem shows, that if a solution of (2.2) exists, it is essentially unique. If there is no solution, there must be some point, which is not interpolated by the rational function. Such a point leads to the indefinite form 0/0, and is called unattainable. This situation occurs when the numerator and denominator polynomial of (2.1) are not relative prime (i.e. they consist of common factors). From now on, it will be assumed that condition (2.2) can be satisfied, and that the rational models don't have unattainable points.

## 2.2 Least squares linearization

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To parameterize the rational model in a least-squares sense, the following nonlinear cost-function needs to be minimized

$$\arg\min_{N,D} \sum_{k=0}^{K} \left| R(s_k) - \frac{\sum_{n=0}^{N} N_n s_k^n}{\sum_{d=0}^{D} D_d s_k^d} \right|^2$$
(2.9)

which equalizes

$$\arg\min_{N,D} \sum_{k=0}^{K} \frac{1}{\left|\sum_{d=0}^{D} D_{d} s_{k}^{d}\right|^{2}} \left| \left(\sum_{d=0}^{D} D_{d} s_{k}^{d}\right) R(s_{k}) - \sum_{n=0}^{N} N_{n} s_{k}^{n} \right|^{2}$$
(2.10)

Unfortunately, the  $D_d$  terms in the denominator which act as a weighting factor, make the least-squares problem non-linear in terms of the parameters, such that it can't be solved analytically. A possible approach is the use of optimization techniques, however they are computationally not very efficient and suffer convergence to local minima. A better alternative, is to solve a (sub-optimal) linearized variation of (2.10), which converges "close enough" to the optimal solution. Possible options, which are commonly used in engineering <sup>[31, 32]</sup> are

1. Kalman's method

$$\arg\min_{N,D} \sum_{k=0}^{K} \left| \left( \sum_{d=0}^{D} D_d s_k^d \right) R(s_k) - \sum_{n=0}^{N} N_n s_k^n \right|^2$$
(2.11)

2. Shanks' method

$$\arg\min_{D} \sum_{k=0}^{K} \left| \left( \sum_{d=0}^{D} D_d s_k^d \right) R(s_k) \right|^2$$
(2.12)

$$\arg\min_{N} \sum_{k=0}^{K} \left| R(s_k) - \frac{\sum_{n=0}^{N} N_n s_k^n}{\sum_{d=0}^{D} D_d s_k^d} \right|^2$$
(2.13)

### 3. Steiglitz-McBride or Sanathanan-Koerner iteration

Solve (2.11) or (2.12) to obtain an initial guess of model parameters D (poles) in iteration t = 0. Set  $D^{(0)} = D$ , and solve (2.10) iteratively <sup>1</sup>

$$\arg\min_{D^{(t)},N^{(t)}} \sum_{k=0}^{K} \frac{1}{\left|\sum_{d=0}^{D} D_{d}^{(t-1)} s_{k}^{d}\right|^{2}} \left| \left(\sum_{d=0}^{D} D_{d}^{(t)} s_{k}^{d}\right) R(s_{k}) - \sum_{n=0}^{N} N_{n}^{(t)} s_{k}^{n} \right|^{2}$$
(2.14)

Due to the linearization, all techniques suffer unbalanced weighting if K + 1 > N + D + 1, however it was shown in <sup>[14, 29]</sup> that iterative least-squares techniques such as the Steiglitz-McBride iteration have favorable convergence properties, compared to Kalman's method or a sequential estimation of the poles and zeros such as Shanks' method. A detailed analysis of these linearizations can be found in literature <sup>[32]</sup>, and will not be repeated here.

Figure 2.1 illustrates the effects of unbalanced weighting, introduced by suboptimal linearization. The reflection coefficient  $S_{11}$  of a multipole filter is sampled very densely (1500 equidistant samples), and is approximated by a rational function with 80 poles. This amount of poles is more than sufficient to obtain an overall accuracy of -65 dB, since this accuracy can be obtained using rational interpolation techniques. This fit was calculated in a least-squares sense using Kalman's method by solving (2.11) in a multiprecision floating point environment with a precision of 1000 bits <sup>[6]</sup>. This approach ensures that all numerical issues are circumvented, and reveals the effects of linearization. Clearly, the accuracy of the fit isn't spread equally over the frequency range of interest, and only an accuracy of -50dB is achieved.

<sup>&</sup>lt;sup>1</sup> In <sup>[13]</sup>, it was proposed to flip unstable poles of the denominator into the left half of the complex plane in each iteration, to achieve Bounded-Input-Bounded-Output models. Afterwards, the numerator expression is calculated to minimize the fitting error. Since the data coming from an LTI system has a physical behaviour, it can be fitted with stable poles. However, this approach will only be successfull when the sampling of the data is dense enough, and the model order is high enough. If an (undersampled) subset of the data is fitted with a lower order model, unstable poles may be needed to approximate the system with sufficient accuracy.



Figure 2.1: Magnitude of data and fit (left), and error of fit (right), based on Kalman linearization & Multiprecision floating-point arithmetic

## SECTION 3 SELECTION OF OPTIMAL BASISFUNCTIONS.

#### 3.1 Power Series

To solve the identification problem, it is desired to satisfy  $R^{(t)}(s_k) = H^{(t)}(s_k)$ for all data samples and frequency derivatives  $(s_k, H^{(t)}(s_k))$ ,  $\forall k = 0, 1, ..., K$  and  $\forall t = 0, 1, ..., T$ . 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 <sup>[24]</sup>. The identification problem is linearized, e.g. using Kalman's method, which leads to the following equations (2.11). At a given complex frequency point  $s_k$ , we get

$$A_k x = b_k \tag{3.1}$$

where

$$A_{k} = \begin{bmatrix} 1 & \dots & s_{k}^{N} & -s_{k}H(s_{k}) & \dots & -s_{k}^{D}H(s_{k}) \end{bmatrix}$$
(3.2)

$$x = \begin{bmatrix} N_0 & \dots & N_N & D_1 & \dots & D_d \end{bmatrix}^T$$
(3.3)

$$b_k = [H(s_k)] \tag{3.4}$$

 $D_0$  can be chosen as 1, since both the numerator and denominator can be divided by the same constant value without loss of generality. A direct solution with real coefficients  $N_n$  and  $D_d$  can be found, by writing out (3.1) for all frequencies  $s_k$ , and solving the following set of linear equations in a least squares sense

$$\begin{bmatrix} \Re(A) \\ \Im(A) \end{bmatrix} x = \begin{bmatrix} \Re(b) \\ \Im(b) \end{bmatrix}$$
(3.5)

When frequency derivatives of the data are available at the discrete frequencies  $s_k$ , (2.2) can be generalized. The coefficients  $N_n$  and  $D_d$  of the rational fitting model now satisfy :

$$H^{(t)}(s_k) \sum_{d=0}^{D} D_d s_k^{d} = \sum_{n=t}^{N} N_n s_k^{n-t} \frac{n!}{(n-t)!}$$

$$-\sum_{m=1}^{t} \sum_{d=m}^{D} {\binom{t}{m}} H^{(t-m)}(s_k) D_d s_k^{d-m} \frac{d!}{(d-m)!}$$
(3.6)

where  $H^{(t)}$  is the t<sup>th</sup> order derivative of the frequency domain data. All derivatives are relative to s. The set of equations at all frequencies  $s_k$  and for all derivatives t, can be written in a similar matrix form as equation (3.5).

Although some of the numerical problems can be relieved by scaling the frequencies <sup>[25]</sup>, the conditioning of this system deteriorates fast when the order of the model increases, or when the frequency range of interest gets more broad.

#### 3.2 Orthogonal Fitting Techniques

Chebyshev polynomials of the first kind

**Definition 3** An inner product  $\langle ., . \rangle$  is a bilinear function of elements  $p_u, p_v, p_w$  of a vector space that satisfies the axioms :

- 1.  $\langle p_u, p_u \rangle \geq 0$  with equality if and only if  $p_u \equiv 0$
- 2.  $\langle p_u, p_v \rangle = \langle p_v, p_u \rangle$
- 3.  $\langle p_u + p_v, p_w \rangle = \langle p_u, p_w \rangle + \langle p_v, p_w \rangle$
- 4.  $\langle \alpha p_u, p_w \rangle = \alpha \langle p_u, p_w \rangle$  for any scalar  $\alpha$

**Definition 4** Two functions  $p_u(x)$  and  $p_v(x)$  in  $L_2[a, b]$ , are said to be orthogonal on the interval [a,b] with respect to a given continuous and non-negative weight function w(x) if

$$\langle p_u(x), p_v(x) \rangle = \int_a^b w(x) p_u(x) p_v(x) dx = 0$$
 (3.7)

**Definition 5** A Chebyshev polynomial  $T_i(x)$  of the first kind is a polynomial in x of degree i, defined by the relation  $T_i(x) = \cos(i\phi)$  when  $x = \cos \phi$ .

From Simpson's rule, it follows that

$$\cos(i\phi) + \cos(i-2)\phi = 2\cos\left(\frac{i\phi + (i-2)\phi}{2}\right) \cdot \cos\left(\frac{i\phi - (i-2)\phi}{2}\right)$$
$$= 2\cos(i-1)\phi\cos\phi$$
(3.8)

This trigonometric identity leads to the fundamental recurrence relation  $T_i(x) = 2xT_{i-1}(x) - T_{i-2}(x)$  together with the initial conditions  $T_0(x) = 1, T_1(x) = x$ .

If the continuous inner product is defined as

$$\langle T_u(x), T_v(x) \rangle = \int_a^b w(x) T_u(x) T_v(x) dx = 0$$
(3.9)

using the interval [a,b] = [-1,1] and weight function  $w(x) = (1-x^2)^{-\frac{1}{2}}$ , then the Chebyshev polynomials of the first kind satisfy  $\langle T_u, T_v \rangle = 0$  if  $u \neq v$ <sup>[21]</sup>.

The numerator and denominator polynomial of the rational function R(s) can be represented as a linear combination of Chebyshev polynomials of the first kind  $T_i(\omega)$  where  $\omega$  represents the angular frequency  $2\pi f$ . The even Chebyshev polynomials consist of even powers of  $\omega$ , while the odd Chebyshev polynomials only consist of odd powers of  $\omega$ . Since the Chebyshev polynomials have real coefficients and a real input variable  $\omega$ , the odd terms are multiplied with complex j.

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n,even} N_n T_n(\omega) + j \cdot \sum_{n,odd} N_n T_n(\omega)}{\sum_{d,even} D_d T_d(\omega) + j \cdot \sum_{d,odd} D_d T_d(\omega)}$$
(3.10)

The identification problem can be linearized, e.g. using Kalman's method, which leads to the following homogenous equations

$$\left(\sum_{d,even} D_d T_d(\omega) + j \sum_{d,odd} D_d T_d(\omega)\right) H(j\omega) = \sum_{n,even} N_n T_n(\omega) + j \sum_{n,odd} N_n T_n(\omega) \quad (3.11)$$

The linear equations are solved for all angular frequencies  $\omega$ , in order to determine the unknown system parameters  $N_n$  and  $D_d$ . To ensure complex conjugacy of the poles and zeros, the real and imaginary part of each equation is separated, as in (3.5). 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 <sup>[23]</sup>. Therefore, the system of equations is usually better conditioned.



Figure 3.1: Power series and Chebyshev polynomials on the interval [0,1]

From (3.9), it follows that the angular frequencies must be scaled and shifted to the unit interval [-1,1] in order to take fully advantage of the orthogonality. Under normal circumstances however, this property can't be satisfied since the transfer function (and consequently also the frequency response) is required to be hermitian symmetric over the real axis. To solve this problem, the frequencies must be scaled into ]0,1], e.g. by dividing all frequencies by  $\omega_{\text{max}}$ . As the poles and zeros of the model are usually desired in terms of the monomial basis, an inverse basis transformation from the Chebyshev polynomials to the power series is required. However, this requires the calculation of the polynomial coefficients, which can be ill-conditioned. Also, the polynomials should be evaluated recursively to obtain best accuracy.

<u>Orthonormal Forsythe Polynomials</u> 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, just as well as on a continuum. <sup>[21]</sup> Forsythe polynomials are formal orthogonal polynomials, which are defined by the following three-term recurrence <sup>[10]</sup>.

$$p_{-1}(f) = 0$$

$$P_{0}(f) = 1$$

$$\dots$$

$$P_{i}(f) = j(2\pi f - \alpha_{i-1})p_{i-1}(f) + \beta_{i-1}p_{i-2}(f)$$
(3.12)

The  $\alpha$  and  $\beta$  coefficients are selected to make the orthogonality conditions hold over the discrete sample set  $\{f_k\}$ 

$$\alpha_i = \frac{\sum_{k=0}^{K} 2\pi f_k(w_k P_i(f_k))(w_k P_i(f_k))^*}{\sum_{k=0}^{K} (w_k P_i(f_k))(w_k P_i(f_k))^*}$$
(3.13)

$$\beta_i = \sqrt{\sum_{k=0}^{K} (w_k P_i(f_k)) (w_k P_i(f_k))^*}$$
(3.14)

and the polynomials are orthonormalized by

$$p_i(f) = \frac{P_i(f)}{\beta_i} \tag{3.15}$$

Summating over all negative and positive sample frequencies, and taking advantage of the fact that  $w_k = w_{-k}^*$ , the following simplified recursive relation ( $\alpha_i=0$ ) is obtained

$$p_{-1}(f) = 0$$

$$P_{0}(f) = 1$$

$$\dots$$

$$P_{i}(f) = j2\pi f p_{i-1}(f) + \beta_{i-1} p_{i-2}(f)$$
(3.16)

where the  $\beta$  coefficients are defined as in (3.14). This way, a simplified formulation of the polynomials is given as

$$p_i(f) = \frac{P_i(f)}{\beta_i} \tag{3.17}$$

Due to the orthonormality, the magnitude of the Forsythe polynomials is normalized in the sample frequencies with respect to the discrete inner product

$$\sum_{\forall k} w_k p_i(f_k) (w_k p_j(f_k))^* = \delta_{ij} \quad \forall 0 \le i, j < K$$
(3.18)

Similar to (3.10), the numerator and denominator polynomial of the rational function R(s) can be represented as a linear combination of generalized Forsythe polynomials <sup>[26]</sup>.

$$R(s) = \frac{N(f)}{D(f)} = \frac{\sum_{n=0}^{N} N_n p_n(f)}{\sum_{d=0}^{D} D_d q_d(f)}$$
(3.19)

 $p_i(f)$  and  $q_i(f)$  are orthonormal with respect to the inner product (3.18), provided that the weighting factor  $w_k$  for the numerator polynomial is set to 1, and the weighting factor for the denominator polynomial is set to  $H(s_k)$ . The identification problem can be linearized, e.g. using Kalman's method, which leads to the following homogenous equations

$$\left(\sum_{d=0}^{D} D_d q_d(f)\right) H(s) = \sum_{n=0}^{N} N_n p_n(f)$$
(3.20)

Let's define the vectors  $U_r, V_r, W$  and the matrices U and V as

$$U_r = [p_r(s_0) \dots p_r(s_K) \ p_r(s_0^*) \dots p_r(s_K^*)]^T$$
(3.21)

$$V_r = [H(s_0)q_r(s_0) \dots H(s_K)q_r(s_K) H^*(s_0)q_r(s_0^*) \dots H^*(s_K)q_r(s_K^*)]^T \quad (3.22)$$

$$U = [U_0 \dots U_N] \text{ and } V = [V_1 \dots V_D]$$
(3.23)

Then the normal equations are obtained as

$$\begin{pmatrix} Y & X \\ X^T & Z \end{pmatrix} \begin{pmatrix} N \\ D \end{pmatrix} = \begin{pmatrix} G \\ F \end{pmatrix}$$
(3.24)

with  $Y = (U^*)^T(U)$ ,  $Z = (V^*)^T(V)$ ,  $X = -\Re((U^*)^T(V))$ ,  $G = \Re((U^*)^T(V_0))$ , and  $F = \Re((V^*)^T(V_0))$ . Due to the orthonormality of the Forsythe polynomials, Y = Z = I, where I represents the identity matrix, and F=0. This way, real coefficients are obtained when following two systems of equations are solved consecutively.

$$(I - (X^T X))D = -X^T G (3.25)$$

$$N = G - XD \tag{3.26}$$

In <sup>[27, 11]</sup>, it is proven that this approach makes the normal equations best conditioned, in a sense that no other polynomial basis can be found resulting in a better conditioned form of the normal equations. Determination of the polynomial coefficients can be ill-conditioned, so although it is time-consuming, a recursive evaluation of the polynomials is required in order to get accurate results. As new samples become available, all orthogonal polynomials need to be recalculated, which is computationally not efficient. Moreover, the technique doesn't extend well to MIMO systems, because the orthogonality of the denominator polynomials depends on the S-parameters.

When frequency derivatives of the data are available, the Forsythe polynomials are generalized. If  $p_i^{(t)}(f_k)$  represents the  $t^{th}$  order derivative of the  $i^{th}$  Forsythe polynomial, evaluated in frequency  $f_k$ , it can be expressed as

$$p_i^{(t)}(f_k) = \frac{t p_{i-1}^{(t-1)}(f_k) + j2\pi f p_{i-1}^{(t)}(f_k) - \beta_{i-1} p_{i-2}^{(t)}(f_k)}{\beta_i}$$
(3.27)

Hence, the coefficients  $N_n$  and  $D_n$  of the rational fitting model now satisfy :

$$H^{(t)}(s_k) \sum_{d=0}^{D} D_d q_d^{(0)}(f_k) = \sum_{n=t}^{N} N_n p_n^{(t)}(f_k)$$

$$-\sum_{m=1}^{t} \sum_{d=m}^{D} {t \choose m} H^{(t-m)}(s_k) D_d q_d^{(m)}(f_k)$$
(3.28)

where  $p_n^{(t)}$  is the  $t^{th}$  order derivative of the  $n^{th}$  order numerator Forsythe polynomial,  $q_d^{(t)}$  is the  $t^{th}$  order derivative of the  $d^{th}$  order denominator Forsythe 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  $f_k$  and for all derivatives t, can be solved in terms of the unknowns  $N_n$  and  $D_d$ . A breakdown of the orthogonality occurs first for i = K-1, when (3.13) fails. This problem can remedied by introducing virtual samples.

A modification of Forsythe's algorithm, due to Clenshaw, is to represent the polynomials by their Chebyshev expansion <sup>[3]</sup>. Although this method is computationally less efficient than the original in terms of arithmetic operations, this form is more concise and convenient in terms of storage requirements.

Lanczos-based Methods A similar approach was made in  $^{[4, 18]}$ . Let's define matrix V and vector H as

$$V_r = [s_0^r \ s_1^r \ \dots \ s_K^r]^T$$
 and (3.29)

$$H = diag(H(s_0), .., H(s_K))$$
(3.30)

Then the identification problem can be formulated in terms of the unknowns, e.g. using Kalman's method, as

$$\begin{pmatrix} V_{0:N} & -HV_{1:D} \end{pmatrix} \begin{pmatrix} N \\ D \end{pmatrix} = (HV_0)$$
 (3.31)

The columns of the Vandermonde matrix V are  $[1,S1,S^21,...,S^r1]$  where  $S=\text{diag}([s_1,s_2,...,s_K])$ 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 generated using a symmetric Lanczos method, which produces the factorization SQ = QT<sup>[28]</sup>. 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 similar to (3.12),

$$p_i(s) = \left(\frac{s - t_{i,i}}{t_{i+1,i}}\right) p_{i-1}(s) - \frac{t_{i-1,i}}{t_{i+1,i}} p_{i-2}(s)$$
(3.32)

To obtain polynomials which satisfy complex conjugate symmetry, it is required that the basis polynomials are orthogonal on both sides of the frequency axis. This corresponds to generating  $K_{r+1}(\tilde{S}, \tilde{I})$  where  $\tilde{S}=\text{diag}([s_1,...,s_K,s_1^*,...,s_K^*])$ ,  $\tilde{H} = diag(H, H^*)$  and  $\tilde{I}$  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 orthogonal polynomial basis is defined by a simplified three-term recurrence relation ( $\tilde{t}_{i,i} = 0$ ), similar to (3.16).

$$p_i(s) = \frac{s}{\tilde{t}_{i+1,i}} p_{i-1}(s) - \frac{\tilde{t}_{i-1,i}}{\tilde{t}_{i+1,i}} p_{i-2}(s)$$
(3.33)

Hence, the coefficients of the rational model

$$R(s) = \frac{N(s)}{D(s)} = \frac{\sum_{n=0}^{N} N_n p_n(s)}{\sum_{d=0}^{D} D_d p_d(s)}$$
(3.34)

are calculated in the orthogonal basis by solving

$$\left(\begin{array}{cc} \tilde{Q}_{0:N} & -\tilde{H}\tilde{Q}_{1:D} \end{array}\right) \left(\begin{array}{c} N \\ D \end{array}\right) = \left(\tilde{H}\tilde{Q}_0\right)$$
(3.35)

Since the dual-basis approach with Forsythe polynomials was optimal in the sense that it makes the normal equations best conditioned, no real breakthrough was achieved with this technique. Furthermore it shares the same advantages and disadvantages, however, using the same basis in numerator and denominator simplifies the extension to MIMO systems with common poles.

When frequency derivatives of the data are available, the orthonormal polynomials are generalized. If  $p_i^{(t)}(s)$  represents the  $t^{th}$  order derivative of the  $i^{th}$  polynomial, evaluated in frequency s, it can be expressed as

$$p_i^{(t)}(s_k) = \frac{t p_{i-1}^{(t-1)}(s_k) + s p_{i-1}^{(t)}(s_k) - \tilde{t}_{i-1,i} p_{i-2}^{(t)}(s_k)}{\tilde{t}_{i+1,i}}$$
(3.36)

Hence, the coefficients  $N_n$  and  $D_n$  of the rational fitting model now satisfy :

$$H^{(t)}(s_k) \sum_{d=0}^{D} D_d p_d^{(0)}(s_k) = \sum_{n=t}^{N} N_n p_n^{(t)}(s_k)$$

$$-\sum_{m=1}^{t} \sum_{d=m}^{D} {t \choose m} H^{(t-m)}(s_k) D_d p_d^{(m)}(s_k)$$
(3.37)

where  $p_n^{(t)}$  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  $D_d$ .

#### 3.3 Vector Fitting

Recently, a new approximation technique was introduced, which fits the frequency response with a causal pole-residue model <sup>[13]</sup><sup>2</sup>.

$$R(s) = \sum_{p=1}^{P} \frac{c_p}{s - a_p} + d$$
(3.38)

H(s) with  $s = j2\pi f$  can be approximated by a rational function, based upon an initial set of P starting poles  $\bar{a}_p$ , multiplied with an unknown function  $\sigma(s)$ . Since  $\sigma(s)$ 

<sup>&</sup>lt;sup>2</sup> To make the order of numerator significantly larger than the order of the denominator, higherorder polynomials terms can be added to the pole-residue form. By interpolating the inverse of the data samples  $H(s_k)$ , the order of numerator and denominator can be interchanged.

is also rational, it can be represented in pole-residue form, which leads to the following augmented problem :

$$\begin{bmatrix} \sigma(s)R(s) \\ \sigma(s) \end{bmatrix} = \begin{bmatrix} \sum_{p=1}^{P} \frac{c_p}{s-\bar{a}_p} + d \\ \sum_{p=1}^{P} \frac{\tilde{c}_p}{s-\bar{a}_p} + 1 \end{bmatrix}$$
(3.39)

The problem can be linearized in terms of the unknowns  $c_p$ , d and  $\tilde{c}_p$  by multiplying the second line of the vector equation (3.39) with R(s).

$$\left(\sum_{p=1}^{P} \frac{c_p}{s - \bar{a}_p} + d\right) = \left(\sum_{p=1}^{P} \frac{\tilde{c}_p}{s - \bar{a}_p} + 1\right) R(s) \tag{3.40}$$

or

$$(\sigma R)_{fit}(s) = \sigma_{fit}(s)R(s) \tag{3.41}$$

Since R(s) should equal H(s) at each frequency sample, we get

$$A_k x = b_k \tag{3.42}$$

where

$$A_k = \begin{bmatrix} \frac{1}{s_k - \bar{a}_1} & \dots & \frac{1}{s_k - \bar{a}_P} & 1 & \frac{-H(s_k)}{s_k - \bar{a}_1} & \dots & \frac{-H(s_k)}{s_k - \bar{a}_P} \end{bmatrix}$$
(3.43)

$$x = \begin{bmatrix} c_1 & \dots & c_P & d & \tilde{c}_1 & \dots & \tilde{c}_P \end{bmatrix}^T$$
(3.44)

$$b_k = \left[ \begin{array}{c} H(s_k) \end{array} \right] \tag{3.45}$$

Writing out (3.42) for all frequencies  $s_k$  gives an overdetermined system of equations :

$$Ax = b \tag{3.46}$$

To ensure that complex conjugacy of the residues, corresponding to complex poles  $\bar{a}_p$  and  $\bar{a}_{p+1}$  is guaranteed, the following modification is performed. Suppose that the poles  $\bar{a}_p$  and  $\bar{a}_{p+1}$  of two partial fractions constitute a complex conjugate pair  $\bar{a}_p = a' + ja'', \bar{a}_{p+1} = a' - ja''$ . Then the corresponding vector columns  $A_{k,p}$  and  $A_{k,p+1}$ of (3.43) can be replaced by

$$A'_{k,p} = \frac{1}{s_k - \bar{a}_p} + \frac{1}{s_k - \bar{a}_p^*} \quad and \quad A'_{k,p+1} = \frac{j}{s_k - \bar{a}_p} - \frac{j}{s_k - \bar{a}_p^*} \tag{3.47}$$

such that the residues  $c_p = c' + jc''$ ,  $c_{p+1} = c' - jc''$  satisfy complex conjugacy as well. This has the effect that the corresponding residues in the solution vector x, become equal to c' and c'' respectively.

To preserve that the coefficients of the rational functions are real, (3.46) is formulated as :

$$\begin{bmatrix} \Re(A) \\ \Im(A) \end{bmatrix} x = \begin{bmatrix} \Re(b) \\ \Im(b) \end{bmatrix}$$
(3.48)

After the parameterization of the rational model, the following function approximations are obtained

$$(\sigma R)_{fit}(s) = \frac{\prod_{p=1}^{P} (s - z_p)}{\prod_{p=1}^{P} (s - \bar{a}_p)} \quad and \quad \sigma_{fit}(s) = \frac{\prod_{p=1}^{P} (s - \tilde{z}_p)}{\prod_{p=1}^{P} (s - \bar{a}_p)} \tag{3.49}$$

From (3.49), R(s) can be calculated

$$R(s) = \frac{(\sigma R)_{fit}(s)}{\sigma_{fit}(s)} = \frac{\prod_{p=1}^{P} (s - z_p)}{\prod_{p=1}^{P} (s - \tilde{z}_p)}$$
(3.50)

The residues of R(s) can be obtained by solving (3.38) with the zeros of  $\sigma(s)$  as new poles for R(s).

When frequency derivatives are available, a modification is performed by deriving the left hand side and right hand side of equation (3.40)<sup>[9]</sup>. This leads to the following system of equations for a certain frequency point  $s_k$ :

$$A_{k} = \begin{bmatrix} \psi_{1,0}(s_{k}) & \dots & \psi_{P,0}(s_{k}) & 1 & \phi_{1,0}(s_{k}) & \dots & \phi_{P,0}(s_{k}) \\ \psi_{1,1}(s_{k}) & \dots & \psi_{P,1}(s_{k}) & 0 & \phi_{1,1}(s_{k}) & \dots & \phi_{P,1}(s_{k}) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \psi_{1,T}(s_{k}) & \dots & \psi_{P,T}(s_{k}) & 0 & \phi_{1,T}(s_{k}) & \dots & \phi_{P,T}(s_{k}) \end{bmatrix}$$
(3.51)

 $x = \begin{bmatrix} c_1 & \dots & c_P & d & \tilde{c}_1 & \dots & \tilde{c}_P \end{bmatrix}^T$ (3.52)

$$b_k = \begin{bmatrix} H^{(0)}(s_k) & H^{(1)}(s_k) & \dots & H^{(T)}(s_k) \end{bmatrix}^T$$
(3.53)

where  $\psi_{p,t}(s_k)$  is defined as

$$\psi_{p,t}(s_k) = \frac{d^t}{ds^t} \left[ (s_k - \bar{a}_p)^{-1} \right] = (-1)^t t! (s_k - \bar{a}_p)^{-(t+1)}$$
(3.54)

and based on Leibniz' identity,  $\phi_{p,t}(s_k)$  represent

$$\phi_{p,t}(s_k) = \frac{d^t}{ds^t} [-H(s_k)(s_k - \bar{a}_p)^{-1}] = -\sum_{\tau=0}^t \begin{pmatrix} t \\ \tau \end{pmatrix} H^{(t-\tau)}(s_k)\psi_{p,\tau}(s_k)$$
(3.55)

To enforce complex conjugacy of poles and residues, a modification similar to (3.47) is performed, by replacing the corresponding column vectors  $A_{k,p}$  and  $A_{k,p+1}$  by  $A'_{k,p} = \psi_{p,t}(s_k) + \psi_{p+1,t}(s_k)$  and  $A'_{k,p+1} = j\psi_{p,t}(s_k) - j\psi_{p+1,t}(s_k)$ .

When the system is solved in a least squares sense, the new poles can be reused as initial starting poles and the fitting process is repeated several times.

Essentially, this method is an "intuitive" reformulation of a Sanathanan-Koerner iteration with rational basis functions <sup>[14,7,15]</sup>.

Suppose the numerator and denominator expression of the rational function is expanded as a linear combination of partial fractions based on common poles, which spans the same space as (3.38).

$$R(s) = \frac{\sum_{p=1}^{P} \frac{c_p}{s - \bar{a}_p} + d}{\sum_{p=1}^{P} \frac{\tilde{c}_p}{s - \bar{a}_p} + 1}$$
(3.56)

Then the identification problem can be linearized using Kalman's method which reduces to the following set of homogenous equations

$$\left(\sum_{p=1}^{P} \frac{c_p}{s - \bar{a}_p} + d\right) - R(s) \left(\sum_{p=1}^{P} \frac{\tilde{c}_p}{s - \bar{a}_p} + 1\right)$$
(3.57)

Note that equation (3.57) reduces exactly to the pole-identification of Vector Fitting (3.40).

Since usually, the poles and residues of the model require less significant digits than the model parameters, more accurate results are achieved than provided by the former techniques. Also, the inversion of a Vandermonde-like matrix, and the use of orthogonal polynomials is avoided by solving a Cauchy-like system of equations. The main disadvantage of the technique, is that the conditioning of (3.46) is highly dependent on the initial choice of starting poles. However, the conditioning often improves when the poles converge. For a detailed analysis of the optimal initial polelocation, the reader is referred to <sup>[13,30]</sup>.

## 3.4 Thiele-type Continued Fractions

The use of continued fractions as rational interpolants in the design of microwave circuits was proposed in <sup>[19]</sup>, and later extended to the multivariate case <sup>[20]</sup>. The rational model can be represented as a convergent of a corresponding Thiele-type continued fraction

$$R_k(s) = H(s_0) + \frac{s - s_0}{\phi_1(s_1, s_0) + \frac{s - s_1}{\phi_2(s_2, s_1, s_0) + \dots + \frac{s - s_{k-1}}{\dots + \frac{s - s_{k-1}}{\phi_k(s_k, s_{k-1}, \dots, s_0)}}}$$
(3.58)

$$= H(s_0) + \sum_{m=1}^{k} \frac{s - s_{m-1}}{|\phi_m(s_m, s_{m-1}..., s_0)|} \text{ for } k = 0, ..., K$$
(3.59)

Each rational expression  $R_k(s)$  is a  $k^{th}$  order partial fraction expansion of (2.1), together constituting a set of interpolants which exhibit increasing accuracy as k increases, reaching a convergent value at k=K. The inverse differences  $\phi_k$ , are the partial denominators of (3.58), and are essentially the coefficients that define  $R_k(s)$ . They are determined recursively from the samples and are defined as follows <sup>[33]</sup>:

$$\phi_1(s_m, s_0) = \frac{s_m - s_o}{H(s_m) - H(s_0)} \tag{3.60}$$

for m = 1, 2, ..., K and

$$\phi_k(s_m, s_{k-1}, \dots s_0) = \frac{s_m - s_{k-1}}{\phi_{k-1}(s_m, s_{k-2}, \dots, s_0) - \phi_{k-1}(s_{k-1}, s_{k-2}, \dots, s_0))}$$
(3.61)

for m = k, k + 1, ..., K and for k = 2, 3, ..., K

The interpolating function  $R_k(s)$  can be evaluated numerically with a three-term recurrence relation

$$N_k(s) = \phi_k(s_k, s_{k-1}, ..., s_0) N_{k-1}(s) + (s - s_{k-1}) N_{k-2}(s) \text{ for } k = 2, 3, ..K(3.62)$$
  

$$D_k(s) = \phi_k(s_k, s_{k-1}, ..., s_0) D_{k-1}(s) + (s - s_{k-1}) D_{k-2}(s) \text{ for } k = 0, 1, ..K(3.63)$$

which is initialized by  $N_0(s) = H(s_0)$ ,  $N_1(s) = \phi_1(s_1, s_0)N_0 + (s - s_0)$ ,  $D_0(s) = 1$ and  $D_1(s) = \phi_1(s_1, s_0)$ . As a consequence of the continued fraction formulation,  $N = D = \frac{k}{2}$  for k even and  $N = \frac{k+1}{2}$  and  $D = \frac{k-1}{2}$  for k odd.<sup>1</sup>

The main advantage of the technique is that it provides numerically accurate results, and interpolates the given dataset. Also, the continued fraction can easily be updated with minimal computational expense, when a new data sample is selected. In <sup>[17]</sup>, a generalization is proposed, which can be applied to fit frequency derivatives. To make the coefficients real-valued, the samples on the negative part of the imaginary axis  $(s_k^*, H^*(s_k))$  should be interpolated as well, such that  $R(s_k^*) = R^*(s_k)$ .

Unfortunately, there are some disadvantages too. This approach based on continued fractions can't be used to approximate the data in a least-squares sense, so the technique fails when the data is contaminated with noise. Also it doesn't extend well to MIMO systems. The conversion from a continued-fraction representation to a ratio of polynomials can imply a loss of accuracy, and successive values of the desired transfer function shouldn't have the same values in order to avoid singularities in the inverse differences. Although the technique provides the ability to precisely specify the frequency response at particular frequencies, it usually causes the response at other frequencies to vary widely from what would be expected. This implies that more samples are needed for smooth functions, compared to least-squares approaches. Also, the model complexity may become excessively large when the sampling of the data is not optimal (too dense).

<sup>&</sup>lt;sup>1</sup> The technique can be extended to more generalized staircases, by combining rational with polynomial interpolation, and interpolating the inverse of the data samples  $H(s_k)$ .

## SECTION 4 NUMERICAL RESULTS

In order to give a fair comparison of the techniques, one should consider which form of representation is most appropriate to represent the final transfer function. The answer to this problem is not straightforward, since some representations are well suited from a mathematical point of view, while engineers may argue that other representations are preferable from a practical perspective. For the sake of argument, it was decided by the authors to represent the transfer function in the form which is numerically most preferable, considering each technique separately.

Figure 4.1 shows the magnitude of the transmission-line coefficient of a lowpass filter over the frequency range of interest [2 GHz - 6 GHz]. To analyze the fitting techniques on this data, an iterative technique is applied. First, an initial set of 4 equidistantly spaced data samples is selected, and rational fitting models are calculated using the different techniques. The transfer function is chosen to be strictly causal (N - 1 = D), and the number of poles is chosen high enough, in order to obtain an interpolating function. This ensures that undesired linearization effects are excluded from the numerical results. In each iteration, the number of equidistant samples is incremented, and the number of iterations was set to 100.



Figure 4.1: Magnitude of data vs. frequency

The equations of the least-squares techniques were solved using Matlab's backslash operator (QR decomposition with column pivoting). Figure 4.2 shows the condition number of the equations which are solved in function of the number of selected samples. Clearly, the numerical conditioning deteriorates fast when the numerator and denominator polynomial of the transfer function are expanded in a power series basis. The other, more advanced techniques, perform significantly better.



Figure 4.2: Condition number of fit vs. number of selected data samples

A close-up of Figure 4.2 is shown in Figure 4.3. When the polynomial basis functions are orthogonalized w.r.t. a continuous inner product (e.g. Chebyshev I, Chebyshev II, or Legendre polynomials), the condition number is very similar, and no real difference can be distinguished. The orthonormalization w.r.t. a discrete inner product (Lanczos) improves the structure of the equations, and leads to a small improvement in numerical conditioning. This can be further optimized, when the numerator and denominator basisfunctions are orthonormalized separately, w.r.t. an appropriate weighting function (Forsythe).

Vector Fitting, on the other hand, uses rational basis functions to estimate the poles and zeros of the fitting model. The algorithm starts from a well-chosen initial set of poles, and was run for 3 iterations. Figure 4.2 and 4.3 shows the condition number of the pole-identification in the final iteration. Before comparing this result to the polynomial fitting techniques, one should keep in mind that this technique estimates

residues of partial fractions, which require less significant digits than coefficients of a polynomial. Therefore a pole-residue model is often a better representation for broadband solutions, since the coefficients of numerator and denominator polynomial may simply not be representable in 16-bit machine precision.



Figure 4.3: Condition number of fit vs. number of selected data samples

The comparison becomes more clear when the fitting error (i.e. the maximal error in the selected data samples) is considered. As can be seen in Figure 4.4, the same conclusions hold for the power series, and orthogonal fitting techniques. Especially interesting is the fitting error of the Vector Fitting technique which is highly accurate (near machine precision), and quite comparable to interpolation techniques based on continued fractions. The main advantage compared to the Tiele CF - approach, is that Vector Fitting can be applied to least-squares solutions, where overdetermined equations need to be solved and the data may be contaminated with noise. Also the pole-residue model is practically more useful and easy to handle, compared to a continued fraction.



Figure 4.4: Accuracy in data samples vs. number of selected data samples

# SECTION 5 CONCLUSIONS

Compact rational macromodels of high-speed passive components, based on fullwave electromagnetic simulation data, are paramount to the success and efficiency of circuit simulation. Solving the rational least-squares approximation problem in a power series basis gives rise to an overdetermined set of highly ill-conditioned equations. A polynomial basis, which is orthogonal w.r.t. a continuous inner product improves the conditioning and the accuracy of the fitting model. The use of a dual basis of orthogonal polynomials, which are orthogonal w.r.t. a discrete inner product with proper weighting improves the structure of the equations, and often gives a small additional advantage at the expense of a higher computational cost. Nevertheless, the advantage of using orthogonal polynomials is often lost, when the rational model needs to be converted into a suitable representation for SPICE-like circuit simulators (e.g. ratio of polynomials, state space representation, or partial fraction expansion). The use of rational bases, combined with iterative least-squares methods, gives rise to a better conditioning and an accuracy which is close to machine precision, and comparable to rational interpolation techniques (Thiele continued fractions). It allows to realize the transfer function as a pole-residue model, which is very fast to evaluate. It doesn't need to be transformed into any other representation, as it can easily be converted into a SPICE netlist.

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