Using efficient multivariate adaptive sampling by minimizing the number of computational electromagnetic analysis needed to establish accurate interpolation models

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***Abstract* — An efficient multivariate adaptive sampling algorithm based on rational interpolation, that establishes accurate surrogate models of microwave circuits, is presented. The technique optimally samples the parameter space in order to minimize the number of CEM analyses, without assuming any *a priori* knowledge of the data. The technique is evaluated on passive microwave structures.**

I. INTRODUCTION

Microwave design incorporating optimization, Monte Carlo analysis or statistical CAD, relies on fast and accurate analyses or models of physical structures to be effective. Computational electromagnetic (CEM) analysis techniques normally provide high accuracy at the expense of computational effort, while circuit models are computationally very effective, but lack wide-band accuracy. Surrogate mathematical models, directly fitting data from CEM simulations, offer fast and accurate solutions to this problem, and are increasingly used in the design of microwave components.

Surrogate interpolation models require only storage of the interpolant coefficients, and in addition normally require smaller data sets than either neural networks or look-up tables to establish a model. While polynomial interpolants are often used, rational functions yield better results for functions containing poles or for meromorphic functions [1]-[9]. Polynomial interpolation is prone to wild oscillations and an acceptable accuracy is sometimes achieved only by polynomials of intolerably high degree [10], [11].

The extension of univariate interpolation to multivariate interpolation is not trivial since a large degree of freedom in the choice for the numerator and denominator polynomials exists. Only a few multivariate sampling algorithms have been published. In [9] the authors use a rectangular grid of support points and recursive univariate interpolation to establish the multidimensional interpolation space. They also mention establishing a multivariate function by solving a linear system of equations. In [7] multivariate polynomials are used to build a model for the geometrical parameters at a single frequency and rational interpolation is used to combine these polynomials to determine the entire interpolation space.

This paper presents two new concepts to minimize the number of support points needed to establish a good model, one in terms of adaptive sampling and the other on interpolation functions. The first is a novel adaptive sampling algorithm for general multivariate interpolation, based on a Thiele-type branched continued fraction representation of a rational function. This is an extension of a recently published adaptive sampling algorithm for the univariate case [12], [13]. To enable more efficient placement of support points, we propose a variation of the standard branched continued fraction that uses approximation to establish a non-rectangular grid of support points. The sampling algorithm is fully automatic, does not require any *a priori* knowledge of the microwave structure under study, and makes no assumptions concerning it. It does not require derivatives, is widely applicable and is in no way restricted to the specific examples shown here. The accuracy of the technique is illustrated by a two-variable and a three-variable example, with errors of smaller than 0.25 % being achieved in both cases.

II. MULTIVARIATE RATIONAL INTERPOLATION

A multivariate rational function with complex variables γ_d, with $d = 1, 2, \cdots, D$, is defined as:

$$\Re(\gamma_1, \gamma_2, \cdots, \gamma_D) = \frac{N(\gamma_1, \gamma_2, \cdots, \gamma_D)}{D(\gamma_1, \gamma_2, \cdots, \gamma_D)} \qquad (1)$$

It can be constructed by calculating the explicit solution of the system of interpolatory conditions, or by starting a recursive algorithm, or by calculating the convergent of a continued fraction [14]. The use of continued fractions as interpolants is a computationally efficient method [15] and

$$\Re(\gamma_1, \gamma_2, \cdots, \gamma_D) = \Re_0(\gamma_2, \gamma_3, \cdots, \gamma_D \,|\, \gamma_1^{(0)}) + \cfrac{\gamma_1 - \gamma_1^{(0)}}{\Re_1(\gamma_2, \gamma_3, \cdots, \gamma_D \,|\, \gamma_1^{(1)}) + \cfrac{\gamma_1 - \gamma_1^{(1)}}{\Re_2(\gamma_2, \gamma_3, \cdots, \gamma_D \,|\, \gamma_1^{(1)}) + \cdots + \cfrac{\gamma_1 - \gamma_1^{(N_1-1)}}{\Re_{N_1}(\gamma_2, \gamma_3, \cdots, \gamma_D \,|\, \gamma_1^{(N_1)})}}} \quad (2)$$

gives accurate numerical results [16], [17] and is therefore used in this paper.

We represent (1) by a Thiele-type interpolating branched continued fraction (BCF) as defined in (2). The partial denominators $\Re_{i_1}(\gamma_2, \gamma_3, \cdots, \gamma_D \,|\, \gamma_1^{(i_1)})$ are multivariate functions, with one less variable than $\Re(\gamma_1, \gamma_2, \cdots, \gamma_D)$ and are defined with γ_1 constant and equal to $\gamma_1^{(i_1)}$. Each partial denominator can be repeatedly substituted by a continued fraction, similar to (2), until the partial denominators become constants. These constants are essentially the coefficients that define the multivariate rational interpolant.

The coefficients of a univariate rational interpolant are defined by a set of inverse differences of the CEM response function that we are trying to model [18]. The univariate interpolant is recursively evaluated using the forward algorithm [19]. Similarly, for the multivariate case the BCF can be evaluated using three-term recurrence relations. Now sets of support points are combined to define sets of univariate rational interpolation functions with D-1 variables constant. The union of these univariate interpolation functions then generates sets of bivariate rational functions. Sets of bivariate functions combine to form three-variable interpolation functions. The process is repeated until a multivariate rational interpolation function with D variables is determined.

It follows that the determination of the coefficients for the multivariate interpolant is equivalent to the determination of coefficients for a set of univariate functions. These univariate functions are determined by repeatedly applying a set of recurrence relations. The general formulation requires that the support points be placed on a fully filled rectangular grid. This constriction, which is an inherent characteristic of BCFs, is not suited for an adaptive sampling algorithm that requires the freedom to choose arbitrary support points in the interpolation space. Furthermore, we expect that a large number of the support points in the grid are redundant. To remove this constriction a variation of the standard BCF is proposed where certain function values are replaced with the previously determined interpolants for those functions. The rectangularly spaced support points required by the BCF can now effectively be calculated from non-rectangularly spaced support points.

II. Adaptive Sampling Algorithm

The determination of an accurate multivariate rational interpolant requires that enough support points, in the case of microwave circuits, normally CEM analyses, be used. In order to calculate the minimum number and the optimal positions of these support points, adaptive sampling for application to the rational function approximation is applied. An estimate of the interpolation error is given by the relative squared error between the current estimate of the interpolant and the previous estimate of the interpolant i.e. before adding the last support point. Starting with a low order interpolant, the technique systematically increases the order by optimally choosing new support points in the areas of highest error, until the required accuracy is achieved. The steps for the multivariate adaptive sampling algorithm are as follows:

1. Using the univariate adaptive sampling algorithm [13], determine a univariate model of each variable γ_d over the interpolation interval, with all other variables set to their midpoint values. In this way, D univariate interpolants, each defined on a line crossing through the center of the interpolation space, are determined.
2. Sort the variable positions in the multivariate interpolant so that the orders N_d of the interpolants determined in step 1 decrease as d increases.
3. Initialize a model with a rectangular grid of support points with three support points along every dimension.
4. Determine a multivariate rational interpolant from the support points.
5. Select a dimension γ_d for selection of new support points. Iterate for $d = D, D\text{-}1, \cdots, 1$.
6. Select a new support point at the maximum of the interpolation error function at γ_d.
7. Renumber the support points so that N_d decreases as d increases.
8. Repeat steps 4 thru 8 until convergence.

II. EXAMPLES

The adaptive sampling algorithm is verified on a two-variable and a three-variable example. To determine the accuracy of the models, they have to be evaluated on an independent evaluation data set, similar to the validation procedures applied to neural networks. In the following examples, the relative squared error E_m between the function and the model on a 30×30 equi-spaced grid for the bivariate case and on a $20 \times 20 \times 20$ equi-spaced grid for the trivariate case, was calculated. Both the maximum and the mean errors in dB are shown for models of varying size. None of these models were reduced in size after a fit was obtained, in contrast to techniques where the order of the interpolant is guessed beforehand, and the interpolation function (calculated by a high number of CEM analyses) is systematically reduced afterwards.

A. Stripline characteristic impedance

A bivariate model $\Re(w/h, \varepsilon_r)$ was determined with the adaptive sampling algorithm for the characteristic impedance $Z_0(w/h, \varepsilon_r)$ of a homogeneous symmetric stripline as shown in Fig. 1. The variables are: the strip width-to-height ratio w/h and the relative dielectric constant ε_r of the substrate. The strip conductor was assumed infinitesimally thin. The model is determined for the parameters $w/h \in [0.05, 1]$ and $\varepsilon_r \in [1, 25]$, which define the interpolation space. At initialization, the 9 chosen support points produce $\Re(w/h, \varepsilon_r)$ with the maximum error equal to -16.4 dB. Table I shows the convergence of the interpolation model using the adaptive sampling algorithm as the number of support points increase. The response $\Re(w/h, \varepsilon_r)$ of the interpolation model with 29 support points and its relative error $E_m(w/h, \varepsilon_r)$, which is less than –56 dB in the interpolation space, are shown in Fig. 2 and Fig. 3 respectively.

TABLE I
CONVERGENCE OF $\Re(w/h, \varepsilon_r)$ FOR THE STRIPLINE EXAMPLE

Number of support points	$E_m(w/h, \varepsilon_r)$ [dB]	
	Mean	Max
9	–29.3	–16.4
14	–33.0	–18.5
21	–42.4	–29.1
29	–72.3	–56.9

TABLE II
CONVERGENCE OF $\Re_{21}(f, a, b)$ FOR THE IRIS EXAMPLE

Number of support points	$E_{21}(f, a, b)$ [dB]	
	Mean	Max
168	–50.0	–18.0
247	–56.9	–19.5
328	–63.2	–31.1
560	–66.5	–33.1
736	–72.7	–52.6

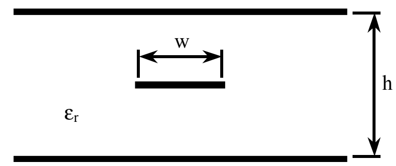

Fig. 1. Cross sectional view of the stripline.

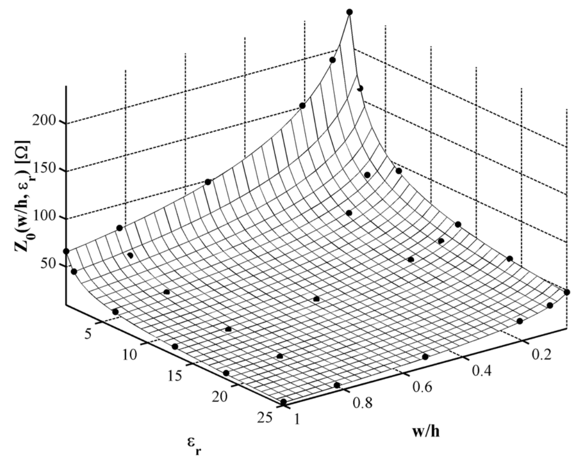

Fig. 2. Response of $\Re(w/h, \varepsilon_r)$ with 29 support points for the stripline example.

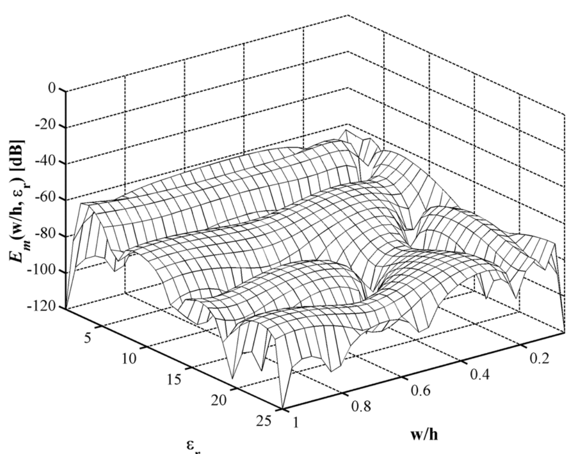

Fig. 3. $E_m(w/h, \varepsilon_r)$ of $\Re(w/h, \varepsilon_r)$ with 29 support points for the stripline example.

B. Iris in rectangular waveguide

A trivariate model $\Re_{21}(f, a, b)$ was determined for the transmission coefficient, i.e. $S_{21}(f, a, b)$ of an iris in a rectangular waveguide as shown in Fig. 4. The variables are: frequency f, gap width a and gap height b. The model was determined for a standard WR90 rectangular waveguide with f ∈ [8 GHz, 12 GHz], a ∈ [8 mm, 15 mm], b ∈ [1 mm, 3 mm] and *l* = 1 mm. The iris is analyzed using the mode matching method [20]. Table II shows the results. An error of smaller than –52 dB in the interpolation space with 736 support points was achieved. This represents excellent performance for a three variable problem in the given interpolation space.

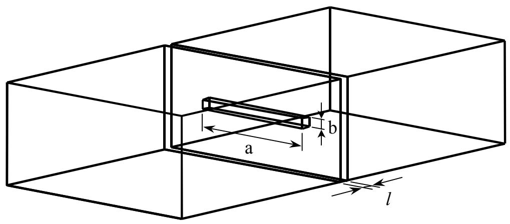

Fig. 4. Iris in rectangular waveguide

V. Conclusion

A fast and efficient adaptive sampling algorithm for multivariate rational interpolation based on the Thiele-type branched continued fraction was presented. Accurate surrogate models with errors of smaller than 0.25 % were determined.

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