

Adaptive Multivariate Rational Data Fitting With Applications in Electromagnetics

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Abstract—The behavior of certain electromagnetic devices or components can be simulated with great detail in software. A drawback of these simulation models is that they are very time consuming. Since the accuracy required for the computational electromagnetic analysis is usually only 2–3 significant digits, an approximate analytic model is sometimes used instead, as noted by Lehmensiek and Meyer in 2001. The most complex model we consider here is a multivariate rational function, which interpolates a number of simulation data. The interpolating rational function is constructed in such a way that it minimizes both the truncation error and the number of simulation data since each evaluation of the simulation model is computationally costly.

Index Terms—Electromagnetics, meta-modeling, multivariate, rational function.

I. INTRODUCTION

WHEN computing a rational interpolant in one variable, all existing techniques essentially yield the same rational function because all rational functions that satisfy the interpolation conditions reduce to the same unique irreducible form. When switching from one to many variables, the situation is entirely different. Not only does one have a large choice of multivariate rational functions, but moreover, different algorithms yield different rational interpolants and apply to different situations.

The rational interpolation of function values that are given at a set of points lying on a multidimensional grid has extensively been dealt with among others in [2]–[6]. In Section III, we describe the situation where the interpolation data are scattered in the multivariate space. This case is far less discussed [7], [8] and proves extremely useful for the application under consideration.

The structured nature of the linear system of equations that determines the coefficients of the rational interpolant leads to severe ill conditioning when using the classical multinomial basis. This is illustrated in Section IV, where we reformulate the problem in terms of an orthogonal polynomial basis. We present a fast solver for the resulting linear system, expressed in the orthogonal basis, which exploits the structure. This solver can cope with the nonsquare block structure of the system and is as stable as Gaussian elimination with partial pivoting.

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In Section V, we discuss related research and illustrate the proposed modeling technique on several higher dimensional examples, real valued, as well as complex valued. In the latter, the additional challenge is to model modulus and argument simultaneously using one and the same set of data points.

To achieve the goals outlined in the abstract, our modeling technique is such that it constructs a rational model as follows.

- Step 1) *Of the most general form*: in the sense that the user can freely choose the terms making up the numerator and denominator polynomial of the rational function, and this in any number of variables.
- Step 2) *Of minimal complexity*: because the data are sampled at optimally located points, without restriction to a grid-like structure, hence reducing the amount of data to be collected and the number of terms in the rational model.
- Step 3) *Of minimal truncation error*: since the algorithm constructs several models of the same complexity, by varying the numerator and denominator degree, and chooses the one with smallest truncation error upper bound.

We also indicate how the rational model can be computed via a fast linear block Cauchy–Vandermonde-like solver, which is a generalization of the algorithm in [9] for use with rectangular blocks.

Step 2) translates to a data updating step, where an additional data point is added and a rational model of higher complexity is fitted, as long as the model is not sufficiently accurate. To this end, an approximation of the truncation error is computed, as we outline later, and the data point at which the estimation of the truncation error is maximal is selected as additional data point.

Step 3) consists of a model updating step, where the degree of the numerator and denominator in the rational model is varied, keeping the sum of the degrees constant, in order to find the rational model with the smallest truncation error upper bound. A rule-of-thumb from univariate approximation theory is that the rational models with an approximately equal numerator and denominator degree are the best choice [10].

We remark that a recursive technique for the computation of the function value of the rational functions in Step 3) is not an option, even though a recursive technique immediately delivers various rational functions of a different degree in the numerator and denominator, which are computed at intermediate steps. Indeed, a recursive technique is useful only if the function value of the desired rational interpolant is required at a small number of points different from the interpolation points. In our application, the rational interpolant needs to be evaluated over an entire high-dimensional grid in order to approximate

the truncation error in Step 2) and to locate the new optimal interpolation point. We, therefore, only focus on a solver for the linear system, which computes the coefficients of the rational model and, hence, yields an explicit representation of the rational function.

II. UNIVARIATE RATIONAL INTERPOLATION AND LOW DISPLACEMENT RANK SYSTEMS

Let the value of the univariate function $f(x)$ be given in the interpolation points $\{x_0, x_1, x_2, \dots\}$, which are noncoinciding. The rational interpolation problem of order (n, m) for f consists of finding polynomials

$$p(x) = \sum_{i=0}^n a_i x^i, \quad q(x) = \sum_{i=0}^m b_i x^i$$

with $p(x)/q(x)$ irreducible and such that

$$f(x_i) = \frac{p}{q}(x_i), \quad i = 0, \dots, S = n + m. \quad (1)$$

In order to solve (1), we rewrite it as

$$f(x_i)q(x_i) - p(x_i) = 0, \quad i = 0, \dots, S = n + m. \quad (2)$$

Condition (2) is a homogeneous system of $S+1$ linear equations in the $S + 2$ unknown coefficients a_i and b_i of p and q and, hence, it has at least one nontrivial solution. It is well known that all the solutions of (2) have the same irreducible form and we shall, therefore, denote by

$$r_{n,m}(x) = \frac{p^*}{q^*}(x)$$

the irreducible form of p/q with p and q satisfying (2) where q^* is normalized according to a chosen normalization. We say that $r_{n,m}$ “interpolates” the given function and by this we mean that p^* and q^* satisfy some of the interpolation conditions (1).

This does not imply that $r_{n,m}$ actually interpolates the given function at all the data because, by constructing the irreducible form, a common factor and, hence, some interpolation conditions, may be cancelled in the polynomials p and q that generate $r_{n,m}$. An interpolation point that appears as a common zero of the numerator and denominator is called an “unattainable” interpolation point.

Since $r_{n,m}$ is the irreducible form, the rational functions p/q with p and q satisfying (2) are called “equivalent.” If the rank of the linear system (2) is maximal, then $r_{n,m} = p^*/q^* = p/q$. In the multivariate case, the issues of unique irreducible form and unattainable interpolation point are much more delicate than in the univariate case.

Let us take a closer look at the linear system of equations (2), defining the numerator and denominator coefficients a_i and

b_i . In the sequel, we assume, for simplicity, but without loss of generality, that this $(S+1) \times (S+2)$ homogeneous linear system of equations can be solved for the choice $b_0 = 1$.

The concept of displacement rank was first introduced in [11] and [12]. We use the definition given in [9] where the displacement rank α of an $(S + 1) \times (S + 1)$ matrix A is defined as the rank of the matrix $LA - AR$ with L and R being the so-called left and right displacement operators. If A is a Cauchy–Vandermonde matrix, as in (2) after choosing $b_0 = 1$, and if all $x_i \neq 0$ and all $|x_i| \neq 1$, then suitable displacement operators are given by $L = \text{diag}(1/x_0, \dots, 1/x_S)$ and $R^T = Z_m^{(1)} \oplus Z_{n+1}^{(1)}$ with

$$Z_k^{(w)} = \begin{pmatrix} 0 & \dots & & 0 & w \\ 1 & 0 & \dots & & 0 \\ 0 & 1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 0 \end{pmatrix}_{k \times k}.$$

The resulting matrix $LA - AR$ then takes the form

$$LA - AR = \begin{pmatrix} f_0(1-x_0^m) & 0 & \dots & 0 & -(1/x_0-x_0^n) & 0 & \dots & 0 \\ \vdots & & & & \vdots & & & \\ f_S(1-x_S^m) & 0 & \dots & 0 & -(1/x_S-x_S^n) & 0 & \dots & 0 \end{pmatrix}.$$

Hence, the displacement rank α of A equals $\alpha = 2$. From a factorization

$$LA - AR = GB \quad G \in \mathbb{C}^{(S+1) \times \alpha} \quad B \in \mathbb{C}^{\alpha \times (S+1)}$$

an LU factorization of the Cauchy matrix $\hat{A} = A(Q_{1,m}^H \oplus Q_{1,n+1}^H)$ can be obtained from [9] with order of complexity $O((S + 1)^2)$. Here, the superscript H denotes complex conjugation and transposition, and the columns of the matrices $Q_{1,m}$ and $Q_{1,n+1}$ contain the eigenvectors of R^T for which explicit formulas are known. By exploiting the displacement structure of the matrix A , the complexity of computing the solution is thus reduced from $O((S + 1)^3)$ to $O((S + 1)^2)$.

When switching from the monomial basis x^i to an orthogonal basis such as, for instance, the Chebyshev polynomials $T_i(x)$, the above technique can be generalized as follows [13]. Here and in the sequel, we use the notation $T_{j,k}$ as a shorthand for $T_j(x_k)$. For A given by

$$A = \begin{pmatrix} f_0 T_{1,0} & \dots & f_0 T_{m,0} & -T_{0,0} & \dots & -T_{n,0} \\ \vdots & & \vdots & \vdots & & \vdots \\ f_S T_{1,S} & \dots & f_S T_{m,S} & -T_{0,S} & \dots & -T_{n,S} \end{pmatrix}$$

and L and R by $L = 2 \operatorname{diag}(x_0, \dots, x_S)$ and $R = Y_m \oplus Y_{n+1}$ with

$$Y_k = \begin{pmatrix} 1 & 1 & & & \\ 1 & 0 & \ddots & & \\ & 1 & \ddots & 1 & \\ & & \ddots & 0 & 1 \\ & & & 1 & 1 \end{pmatrix}_{k \times k}$$

the matrix $LA - AR$ can be factored as GB with the equations shown at the bottom of this page. The displacement rank of the latter A is 4 instead of 2. From the fact that the matrix Y_k can be factored as $Y_k = C_k D_k C_k^T$ where the orthogonal matrix C_k is the discrete cosine transform

$$\begin{aligned} C_k &= (c_{ij})_{k \times k} \\ c_{ij} &= \gamma_i \cos \frac{(i-1)(2j-1)\pi}{2k} \\ \gamma_1 &= \sqrt{1/k} \\ \gamma_{i>1} &= \sqrt{2/k} \end{aligned}$$

and the diagonal matrix D_k is given by

$$D_k = \operatorname{diag} \left(1, \cos \left(\frac{\pi}{k} \right), \dots, \cos \left(\frac{\pi(k-1)}{k} \right) \right) \quad (3)$$

a factorization $LA - AR = GB$ can be transformed into a factorization of $L(AC) - (AC)D$ where $C = C_m \oplus C_{n+1}$, $D = D_m \oplus D_{n+1}$, and AC is a Cauchy-like matrix

$$LA - AR = GB \Rightarrow L(AC) - (AC)D = G(BC).$$

Again, when AC is a Cauchy-like matrix, a fast LU factorization technique for AC can be obtained from [9], leading to a fast LU factorization of A . Similar factorizations exist for other orthogonal polynomial bases [13].

III. SCATTERED MULTIVARIATE RATIONAL INTERPOLATION

Although the situation between one and more variables is substantially different, there is no loss in generality by describing the bivariate case instead of the general higher dimensional case. Let the bivariate function $f(x, y)$ be given in the set of points $\{(x_k, y_k) | 0 \leq k \leq S = n + m\}$ and let us assume that none of the points (x_k, y_k) coincide. Let N (from the ‘‘numerator’’) and

D (from the ‘‘denominator’’) be two finite subsets of \mathbb{N}^2 with which we associate the bivariate polynomials

$$p(x, y) = \sum_{(i,j) \in N} a_{ij} x^i y^j, \quad \#N = n + 1 \quad (4a)$$

$$q(x, y) = \sum_{(i,j) \in D} b_{ij} x^i y^j, \quad \#D = m + 1. \quad (4b)$$

The multivariate rational interpolation problem consists in finding polynomials $p(x, y)$ and $q(x, y)$ with $p(x, y)/q(x, y)$ irreducible such that

$$f(x_k, y_k) = \frac{p}{q}(x_k, y_k), \quad k = 0, \dots, S = n + m. \quad (5)$$

In applications where adaptive sampling is used and data points are placed at optimally located positions, it is an exception rather than the rule that some data points have the same x - or y -coordinates. Hence, techniques available for a grid-like set of data points, such as in [2]–[6], cannot be used. In the sequel, we shall deal with the more general and less-studied multivariate situation where the data set is not necessarily grid structured. We do, however, require that the sets N and D satisfy the inclusion property, meaning that if the index tuple (k, ℓ) belongs to N (or D), then (i, j) also belongs to N (or D) for all $i \leq k$ and $j \leq \ell$, which is not a severe restriction.

The fact that the numerator and denominator polynomials can be chosen freely by picking the terms $x^i y^j$ in (4) implies that all kinds of situations can be handled. One can opt for a model that is purely polynomial in some variables and rational in the other ones, or a model that takes into account terms of different order (degree) for different variables.

Problem (5) of interpolating the data is reformulated as

$$f(x_k, y_k) \left(\sum_{(i,j) \in D} b_{ij} x_k^i y_k^j \right) - \left(\sum_{(i,j) \in N} a_{ij} x_k^i y_k^j \right) = 0, \quad k = 0, \dots, S = n + m. \quad (6)$$

The set of polynomial tuples $(p(x, y), q(x, y))$ satisfying (6) is denoted by $[N/D]_{n+m}$. In the sequel, we assume that the linear system resulting from (6) has a maximal rank. All rational functions belonging to the set $[N/D]_{n+m}$ are then equal up to a multiplicative constant and lead to the same unique irreducible form. In this case, we represent $[N/D]_{n+m}$ by its (suitably normalized) irreducible form which we denote by $r_{n,m}(x, y)$. For a

$$G = \begin{pmatrix} f_0(1-x_0) & f_0(T_{m+1,0} - T_{m,0}) & x_0 - 1 & T_{n,0} - T_{n+1,0} \\ \vdots & \vdots & \vdots & \vdots \\ f_S(1-x_S) & f_S(T_{m+1,S} - T_{m,S}) & x_S - 1 & T_{n,S} - T_{n+1,S} \end{pmatrix}$$

$$B = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \dots & 0 & 1 \end{pmatrix}_{2 \times m} \oplus \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \dots & 0 & 1 \end{pmatrix}_{2 \times (n+1)}$$

TABLE I
TABLE OF MULTIVARIATE RATIONAL INTERPOLANTS

$r_{0,0}(x, y)$	$r_{0,1}(x, y)$	$r_{0,2}(x, y)$...
$r_{1,0}(x, y)$	$r_{1,1}(x, y)$	$r_{1,2}(x, y)$...
$r_{2,0}(x, y)$	$r_{2,1}(x, y)$	$r_{2,2}(x, y)$...
\vdots	\vdots	\vdots	\ddots

discussion of the nonuniqueness of the rational interpolant, we refer to [14].

When $q(x_k, y_k) \neq 0$ for all data points, then no interpolation points are unattainable. Note that, in the multivariate case, unattainability can also occur if $q(x_k, y_k) = 0 = p(x_k, y_k)$ without $p(x, y)$ and $q(x, y)$ having a common factor. In the numerical examples, we guard against unattainability by monitoring the location of the zeroes of the denominator.

When modeling real-life examples, usually a sequence of consecutive approximants is computed. The rational functions $r_{n,m}(x, y)$ can be ordered in a two-dimensional table as indicated in Table I.

From univariate rational approximation theory [10], we know that for some classes of functions, the most accurate rational models with the smallest truncation error are the ones with approximately equal numerator and denominator degrees. Although, to this day, this fact has only partially been proven for the multivariate case [15], we use it as a rule-of-thumb in our algorithm to update the interpolating rational function.

With the same set of datapoints $\{(x_k, y_k) | k = 0, \dots, S\}$, one can compute all rational models $r_{n,m}(x, y)$ with $n + m = S$, which make up the upward sloping diagonal in Table I from $r_{S,0}(x, y)$ to $r_{0,S}(x, y)$. Assuming that the models near the main diagonal of Table I are the more accurate ones, we associate a penalty with the off-diagonal approximants. Let us denote the target threshold for the relative error in the final model by ϵ . A rational approximant $r_{n,m}(x, y)$ that is off the diagonal in Table I by $d = \lceil S/2 \rceil - m$ is then assigned a penalty error $\mathcal{P}(r_{n,m}) = |s \times d \times \epsilon| \%$ where s is a small integer. In our examples, we have used $s = 2$. The idea is that an off-diagonal approximant is only preferred as a model if its relative truncation error is at least \mathcal{P} better than the truncation error of the diagonal approximant. Another motivation for keeping the approximant close to the diagonal is the following.

It is clear that the relative truncation error of the multivariate rational interpolant must be estimated instead of computed. Indeed, the latter would require that the given function is evaluated in a lot of points in the multidimensional domain of interest, which is precisely what we want to avoid since each evaluation of $f(x, y)$ is very costly. Therefore, the relative error of interest is approximated as follows.

Let $R_p(x, y)$ be the best rational approximant on the diagonal $\{r_{S-1-m,m}(x, y) | m = 0, \dots, S-1\}$ in Table I and let

$$E_m(x, y) = 20 \log_{10} \frac{|r_{S-m,m}(x, y) - R_p(x, y)|}{1 + |r_{S-m,m}(x, y)|}. \quad (7)$$

$R_\ell(x, y)$ is then the best approximant on the diagonal $\{r_{S-m,m}(x, y) | m = 0, \dots, S\}$ in Table I if

$$E_\ell(x, y) + \mathcal{P}(R_\ell) = \min_{m=0, \dots, S} (E_m(x, y) + \mathcal{P}(r_{S-m,m})) \quad (8)$$

Without penalty $\mathcal{P}(r_{n,m})$, the numerator and denominator degrees of $R_\ell(x, y)$ and $R_p(x, y)$ may vary too much and one can end up with quite incomparable functions $R_\ell(x, y)$ and $R_p(x, y)$ where the former is, for instance, purely polynomial and the latter purely rational.

In practice, for the actual computation of the error estimate $E_m(x, y)$, the multidimensional domain G is discretized and (7) is evaluated at all the grid points of the discretized domain G_Δ . Once $R_\ell(x, y)$ is determined among all rational interpolants on the diagonal based on (8), the grid point at which the (modulus or absolute value of the) error estimate $E_\ell(x, y)$ attains a (discrete) maximum is selected as the additional interpolation point indexed $S+1$. This approach can be replaced by an actual optimization algorithm that searches for the true maximum, but such a decision is left to the user and depends on the dimension of the problem. In the examples of Section V, we compare

$$\max_{(x,y) \in G_\Delta} E_\ell(x, y) \leq \epsilon \quad (9)$$

where ϵ , which is measured in decibels, is typically in the range of -60 . As soon as (9) is satisfied, no interpolation points are added anymore and $R_\ell(x, y)$ is accepted as the final model for $f(x, y)$.

IV. COMPLEXITY AND CONDITIONING

Let us introduce the notation

$$\begin{aligned} I^{(N)} &= \max \{i | (i, j) \in N\} \\ J^{(N)} &= \max \{j | (i, j) \in N\} \\ I^{(D)} &= \max \{i | (i, j) \in D\} \\ J^{(D)} &= \max \{j | (i, j) \in D\}. \end{aligned}$$

Let $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ equal $J^{(N)}$ or $J^{(D)}$ and let us introduce the shorthand notation $\nu = I^{(N)}$ and $\delta = I^{(D)}$. Since both N and D satisfy the inclusion property, we can decompose the sets as follows:

$$\begin{aligned} N &= N^{(0)} \cup \dots \cup N^{(\nu)} \\ N^{(i)} &= \{(i, j) | 0 \leq j \leq M_i^{(N)}\} \\ M_i^{(N)} &= \max \{j | (i, j) \in N\} \\ D &= D^{(0)} \cup \dots \cup D^{(\delta)} \\ D^{(i)} &= \{(i, j) | 0 \leq j \leq M_i^{(D)}\} \\ M_i^{(D)} &= \max \{j | (i, j) \in D\}. \end{aligned}$$

This is illustrated in Fig. 1. If $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is attained in the i -direction instead of in the j -direction, then the sets N and D are decomposed horizontally instead of vertically. We point out to the reader that the sequel does not apply if both

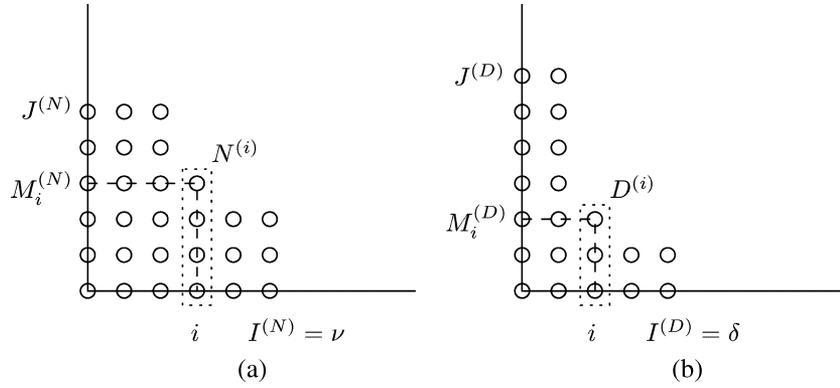


Fig. 1. Decomposition of the index sets N and D . (a) Breaking up N . (b) Breaking up D .

sets N and D are not decomposed in the same way, either both horizontally or both vertically.

Using this notation, we arrange the unknown coefficients a_{ij} and b_{ij} as

$$\begin{aligned} \mathcal{B}^T &= \left(b_{00}, \dots, b_{0, M_0^{(D)}} \mid b_{10}, \dots, b_{1, M_1^{(D)}} \mid \dots \mid \right. \\ &\quad \left. \times b_{\delta 0}, \dots, b_{\delta, M_\delta^{(D)}} \right) \\ \mathcal{A}^T &= \left(a_{00}, \dots, a_{0, M_0^{(N)}} \mid a_{10}, \dots, a_{1, M_1^{(N)}} \mid \dots \mid \right. \\ &\quad \left. \times a_{\nu 0}, \dots, a_{\nu, M_\nu^{(N)}} \right). \end{aligned}$$

Introducing the matrices $C_i^{(D)}$ of size $(S + 1) \times (M_i^{(D)} + 1)$ and the matrices $C_i^{(N)}$ of dimension $(S + 1) \times (M_i^{(N)} + 1)$, respectively, given by

$$\begin{aligned} C_i^{(D)} &= \left(f_k x_k^i \quad f_k x_k^i y_k \quad \dots \quad f_k x_k^i y_k^{M_i^{(D)}} \right)_{k=0, \dots, S} \\ C_i^{(N)} &= \left(-x_k^i \quad -x_k^i y_k \quad \dots \quad -x_k^i y_k^{M_i^{(N)}} \right)_{k=0, \dots, S} \end{aligned}$$

the system of interpolation conditions (6) becomes

$$\begin{pmatrix} C_0^{(D)} & \dots & C_\delta^{(D)} & C_0^{(N)} & \dots & C_\nu^{(N)} \end{pmatrix} \begin{pmatrix} \mathcal{B} \\ \mathcal{A} \end{pmatrix} = 0.$$

Again, without loss of generality, we solve this system with b_{00} normalized to 1. We denote by A the coefficient matrix of the square inhomogeneous linear system, which results from removing the first unknown from \mathcal{B} and the first column from $C_0^{(D)}$.

For Example 2, which is worked out in detail in Section V, we list the ℓ_2 -condition number $\kappa_2(A)$ of A in Table II. Here, $N = N_n$ and $D = D_m$ consist, respectively, of the first $n + 1$ and first $m + 1$ index tuples from the set \mathbb{N}^2 enumerated as

$$\begin{aligned} \mathbb{N}^2 &= \{(0, 0), (1, 0), (0, 1), (2, 0), (0, 2), (1, 1), \\ &\quad (3, 0), (0, 3), (2, 1), (1, 2), \dots\}. \end{aligned}$$

This enumeration makes a maximal number of the index sets N and D symmetric with respect to the variables x and y . In the absence of any information about nonsymmetry of the function $f(x, y)$, which is to be approximated, this is the more appropriate choice.

TABLE II
CONDITIONING IN DIFFERENT BASES

dim(A)	$x^i y^j$	$T_i(x)T_j(y)$	$L_i(x)L_j(y)$
13	6.5e+07	1.2e+04	1.3e+04
18	9.7e+07	2.1e+04	2.2e+04
23	7.6e+09	3.4e+04	3.6e+04
28	1.7e+11	3.4e+04	3.5e+04
33	4.8e+10	8.5e+05	7.6e+05
38	2.7e+12	1.0e+06	1.1e+06
43	1.1e+14	1.9e+06	2.2e+06

It is clear that the problem becomes extremely ill conditioned as the size of the linear system grows. We, therefore, reformulate the multivariate rational data fitting problem in terms of a product form orthogonal basis, such as the product $T_i(x)T_j(y)$ of the Chebyshev polynomials or the product $L_i(x)L_j(x)$ of the Legendre polynomials, instead of the multinomial basis $x^i y^j$. Since the index sets N and D satisfy the inclusion property, this is possible. It suffices to replace each $x_k^i y_k^j$ occurring in (6), as well as in $C_0^{(D)}, \dots, C_\delta^{(D)}$ and $C_0^{(N)}, \dots, C_\nu^{(N)}$ either by $T_i(x_k)T_j(y_k)$ or $L_i(x_k)L_j(y_k)$. If the data points lie outside the hypercube $[-1, 1] \times [-1, 1]$, then an additional change of variables needs to be performed because the orthogonality of the univariate basis factors is only assured on $[-1, 1]$. In Table II, the new condition numbers can be found. It is easy to see that the conditioning of the problem is greatly improved. For Gaussian elimination with partial pivoting applied to the full matrix A , the relative error in the computed solution is typically of the order of the product of the condition number of A and machine epsilon. It can be shown that the fast LU factorization with partial pivoting, which takes into account the displacement structure of A , has the same property under appropriate conditions. This is, in fact, an optimal result for a fast linear system solver. For instance, when computing the solution of the linear system of dimension 40 in Example 2 in double precision (machine epsilon $\approx 10^{-15}$), the solution may not have any significant digits when using the monomial basis (condition number $\approx 10^{14}$), while full single precision accuracy (relative error $\leq 10^{-8}$) is guaranteed when using an orthogonal basis (condition number $\approx 10^6$).

In order to generalize the fast Cauchy–Vandermonde-like solver given in [13], we need to construct block versions of

the left and right displacement operators. We continue with the Chebyshev basis, although similar results can be obtained with the Legendre basis. With $L = 2 \text{diag}(y_0, \dots, y_S)$, the diagonal matrix D_k given by (3) and

$$D = D_{M_0^{(D)}-1} \oplus \left(\bigoplus_{i=1}^{\delta} D_{M_i^{(D)}} \right) \oplus \left(\bigoplus_{i=0}^{\nu} D_{M_i^{(N)}} \right)$$

$$C = C_{M_0^{(D)}-1} \oplus \left(\bigoplus_{i=1}^{\delta} C_{M_i^{(D)}} \right) \oplus \left(\bigoplus_{i=0}^{\nu} C_{M_i^{(N)}} \right)$$

it is easy to see that the resulting $(S+1) \times (S+1)$ matrix $L(AC) - (AC)D$ can be factored as follows:

$$L(AC) - (AC)D = (G_1 \ G_2)(BC) \quad (10)$$

where the k th row ($k = 0, \dots, S$) of the $(S+1) \times (2\delta+2)$ and $(S+1) \times (2\nu+2)$ submatrices G_1 and G_2 are given by

$$G_{1,k} = f_k \left(1 - y_k |T_{M_0^{(D)}+1}(y_k) - T_{M_0^{(D)}}(y_k)| \right. \\ \left. T_1(x_k)(1 - y_k) \right. \\ \left. T_1(x_k) \left(T_{M_1^{(D)}+1}(y_k) - T_{M_1^{(D)}}(y_k) \right) \right| \dots \\ \left. T_\delta(x_k)(1 - y_k) \right. \\ \left. T_\delta(x_k) \left(T_{M_\delta^{(D)}+1}(y_k) - T_{M_\delta^{(D)}}(y_k) \right) \right)$$

$$G_{2,k} = \left(y_k - 1 |T_{M_0^{(N)}}(y_k) - T_{M_0^{(N)}+1}(y_k)| \dots \right. \\ \left. T_\nu(x_k)(y_k - 1) \right. \\ \left. T_\nu(x_k) \left(T_{M_\nu^{(N)}+1}(y_k) - T_{M_\nu^{(N)}}(y_k) \right) \right)$$

and the matrix B consists of zeroes with the exception of the following entries:

ℓ	column number	row number
0	1	1
$1, \dots, \delta$	$-1 + \sum_{i=1}^{\ell} (M_{i-1}^{(D)} + 1)$	2ℓ
	$\sum_{i=1}^{\ell} (M_{i-1}^{(D)} + 1)$	$2\ell + 1$
0	$m + 1$	$2\delta + 2$
$1, \dots, \nu$	$m - 1 + \sum_{i=1}^{\ell} (M_{i-1}^{(N)} + 1)$	$(2\delta + 2) + \ell$
	$m + \sum_{i=1}^{\ell} (M_{i-1}^{(N)} + 1)$	$(2\delta + 2) + (\ell + 1)$

When $\max(I^{(N)}, J^{(N)}, I^{(D)}, J^{(D)})$ is either $I^{(N)}$ or $I^{(D)}$ and N and D are being decomposed horizontally, then L is replaced by $L = 2 \text{diag}(x_0, \dots, x_S)$. Since the matrix AC is a Cauchy-like matrix, the displacement rank technique proposed in [9] can be applied. As mentioned, it incorporates partial pivoting while its order of complexity for the problem under consideration is $O(2(\nu + \delta)(S + 1)^2)$. This is noticeably smaller than that of classical Gaussian elimination as soon as $2(\nu + \delta) \ll S$. The procedure to compute the LU factorization of AC directly from the matrix factors G and BC is fully detailed in [9]. Roughly speaking, all entries in the LU factors can be computed from the scalar products of the rows in G and the columns in BC , and the differences of the entries in the left and right displacement operators L and D .

TABLE III
STRIPLINE CHARACTERISTIC IMPEDANCE

n, m	$\kappa_2(A)$	max	mean	S for [23]	max	mean
3, 3	$7.6e+03$	-16.4	-42.9	9	-16.4	-29.3
4, 6	$1.1e+05$	-30.0	-77.3	14	-18.5	-33.0
9, 9	$7.0e+05$	-43.7	-68.1	21	-29.1	-42.4
14, 10	$1.2e+07$	-71.7	-102.3	29	-56.9	-72.3

V. NUMERICAL ILLUSTRATION

Microwave circuits are used in many electronic sensors such as wireless transmitters or receivers of handheld telephones, antennas, microphones, infrared detectors used in motion sensors, remote-control devices, and photocells to mention just a few. Hence, there is an increasing demand in designing microwave circuits using computer-aided design (CAD) tools. The design techniques include computational electromagnetic (CEM) analysis, lookup tables, and artificial neural networks [16], [17], each with their own drawbacks.

The use of lookup tables necessitates the generation and storage of data points in a database. The amount of storage space increases exponentially with the dimension since the data points are determined in a grid-like nonadaptive way throughout the multidimensional parameter space. The number and location of these data points may, therefore, not be optimal. This can lead to inaccurate modeling, as well as to oversampling. In between the grid points, simple low-order interpolation techniques are used and, hence, only mild fluctuations in the design can be handled.

Artificial neural networks can learn from data, are easy to implement, and also fast to evaluate. Once properly trained, they have the ability to model multidimensional nonlinear functions. The size of the network does not increase exponentially with the dimension. However, neural nets must have the right topology and may require lots of training and testing on a multitude of examples.

To overcome the drawbacks of the above methods, interpolation techniques for circuit optimization are proposed in [18]–[21]. These techniques, when compared with artificial neural networks, normally require the smallest amount of data (obtained from CEM) to establish a useful model. In [22], a rectangular grid of data points is used to construct the multidimensional interpolating model. The sampling algorithm presented in [23] to model standard microwave circuits using multivariate rational interpolating functions is based on a Thiele-type branched continued fraction representation. This interpolation technique also requires that the datapoints in the multivariate space are grid structured, a drawback that is overcome in this paper.

We take our examples from [23] and show that the number of data required for the computation of the model is reduced significantly by means of the new technique that allows the datapoints to be scattered in the interpolation space. All examples are modeled making use of the Chebyshev product basis. In all examples, we list for each computed interpolant $r_{n,m}$ the following:

- n and m , from which the number of datapoints $S + 1 = n + m + 1$ interpolated by $r_{n,m}$ can be determined;

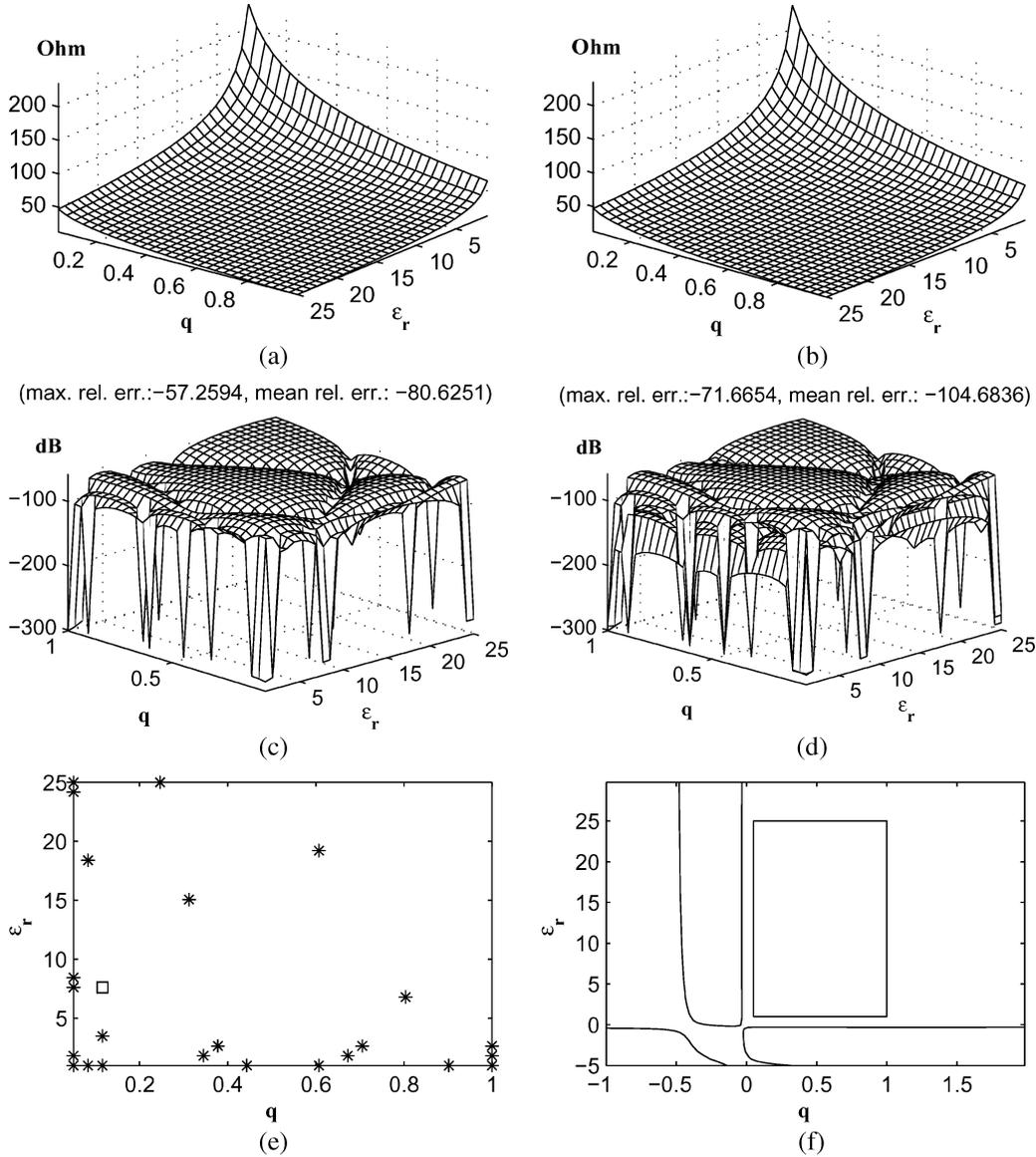


Fig. 2. Model of the stripline characteristic impedance $Z_0(q, \epsilon_r)$. (a) $Z_0(q, \epsilon_r)$. (b) $r_{14,10}(q, \epsilon_r)$. (c) $|Z_0(q, \epsilon_r) - r_{14,10}(q, \epsilon_r)| / (1 + |Z_0(q, \epsilon_r)|)$. (d) $|r_{14,10} - r_{13,10}(q, \epsilon_r)| / (1 + |r_{14,10}(q, \epsilon_r)|)$. (e) Datapoints for $Z_0(q, \epsilon_r)$. (f) Zeroes of denominator of $r_{14,10}(q, \epsilon_r)$.

- condition number $\kappa_2(A)$;
- $\max_{(x,y) \in G_\Delta} E_m(x, y)$, and we compare this to the value for the maximum in [23];
- $\text{mean}_{(x,y) \in G_\Delta} E_m(x, y)$, which is also compared to the value obtained in [23];
- number of datapoints required by the method laid out in [23] to achieve a similar accuracy.

In Example 1, we model the stripline characteristic impedance $Z_0(q, \epsilon_r)$ by a bivariate rational interpolant. The strip width-to-height ratio q is limited to $0.05 \leq q \leq 1$, while the relative dielectric constant ϵ_r lies in the interval $1 \leq \epsilon_r \leq 25$. The results can be found in Table III and Fig. 2. In Fig. 2(a), the function $f(x, y) = Z_0(q, \epsilon_r)$ is graphed, in Fig. 2(b), the rational interpolant $r_{14,10}(q, \epsilon_r)$, in Fig. 2(c), the true relative error $|Z_0(q, \epsilon_r) - r_{14,10}(q, \epsilon_r)| / (1 + |Z_0(q, \epsilon_r)|)$, and in Fig. 2(d), the estimated relative error $|R_\ell(q, \epsilon_r) - R_p(q, \epsilon_r)| / (1 + |R_\ell(q, \epsilon_r)|)$ with $R_\ell(q, \epsilon_r) = r_{14,10}(q, \epsilon_r)$ and $R_p(q, \epsilon_r) = r_{13,10}(q, \epsilon_r)$.

TABLE IV
TRANSMISSION COEFFICIENT OF INDUCTIVE POSTS
IN RECTANGULAR WAVEGUIDE

n, m	$\kappa_2(A)$	max	mean	S for [23]	max	mean
10, 11	$1.8e+04$	-38.3	-61.8	23	-42.6	-59.1
11, 16	$3.4e+04$	-53.5	-77.6	30	-27.4	-52.1
16, 18	$5.7e+05$	-58.5	-81.9	51	-51.3	-76.8
19, 20	$1.6e+06$	-69.1	-88.9	57	-72.5	-87.9

This fairly simple example mainly illustrates that, with the same number of data, the new method can do quite a lot better. With only 25 datapoints (instead of 29 in [23]), a mean error is achieved of less than -100 dB (compared to -70 dB in [23]) and a maximal error of less than $\epsilon = -70$ dB (as opposed to $\epsilon = -55$ dB in [23]). In Fig. 2(e), the datapoints from the interpolation space $[0.05, 1] \times [1, 25]$ that were used to construct $R_\ell(q, \epsilon_r)$ are indicated by an asterisk. The role of the

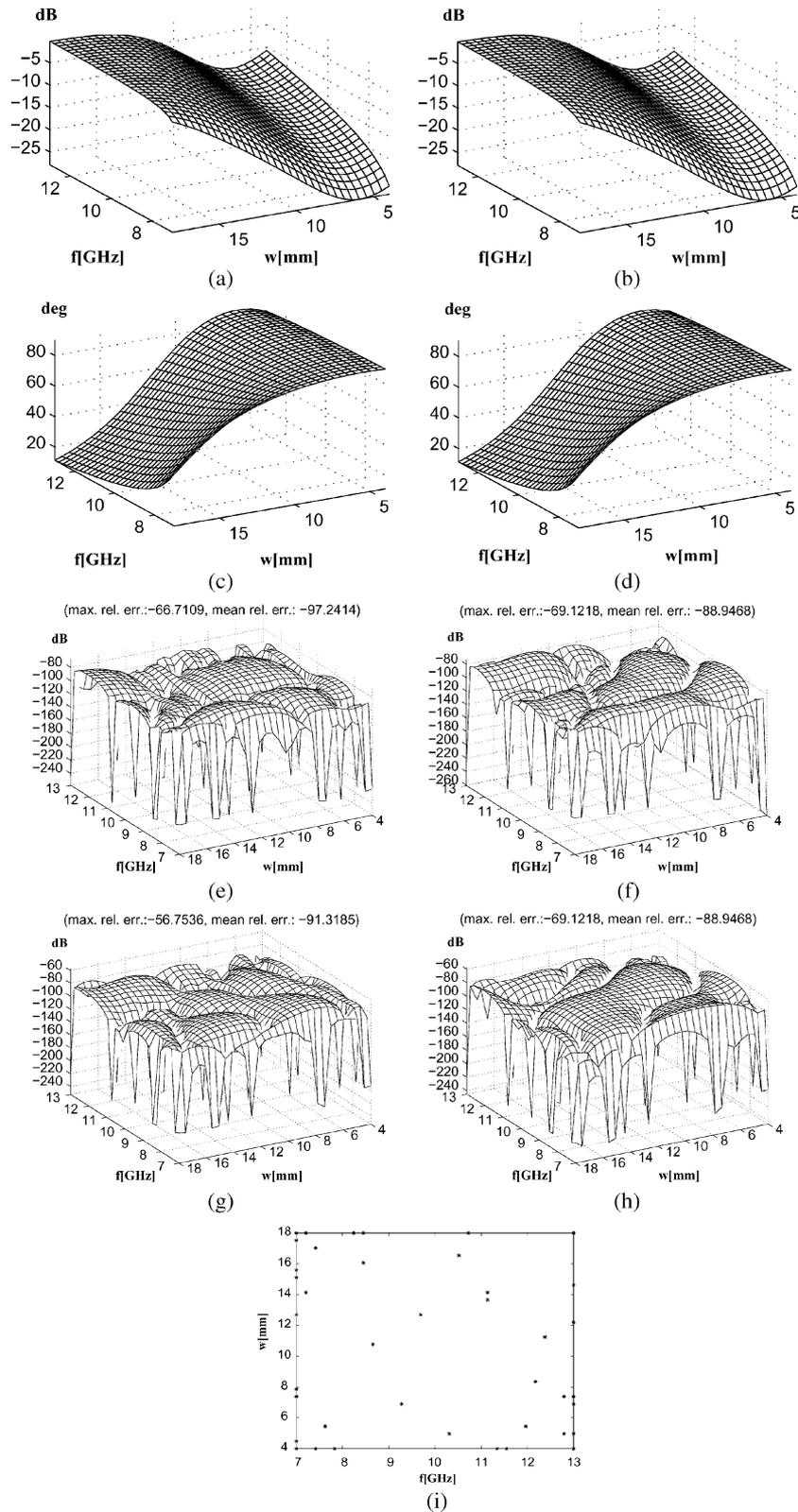


Fig. 3. Model of the transmission coefficient $S_{21}(f, w)$ of two inductive posts in rectangular waveguide. (a) $|S_{21}(f, w)|$. (b) $|r_{19,20}(f, w)|$. (c) $\arg(S_{21}(f, w))$. (d) $\arg(r_{19,20}(f, w))$. (e) $\frac{||S_{21}| - |r_{19,20}||}{(1 + |S_{21}|)}$. (f) $\frac{||\arg r_{19,20}| - |\arg r_{16,22}||}{(1 + |\arg r_{19,20}|)}$. (g) $\frac{|\arg S_{21} - \arg r_{19,20}|}{(1 + |\arg S_{21}|)}$. (h) $\frac{|\arg r_{19,20} - \arg r_{16,22}|}{(1 + |\arg r_{19,20}|)}$. (i) Datapoints for $S_{21}(f, w)$.

denominator zeroes is clear from Fig. 2(f): in the neighborhood of where the slope of the function $Z_0(q, \epsilon_r)$ becomes steeper,

the rational model places poles. The interpolation space is delimited by a rectangle.

TABLE V
CAPACITIVE STEP IN RECTANGULAR WAVEGUIDE: REFLECTION COEFFICIENT

n, m	$\kappa_2(A)$	max	mean	S for [23]	max	mean
3, 14	$3.1e+03$	-24.7	-40.4	343	-15.3	-55.5
7, 16	$4.6e+03$	-30.8	-49.0	593	-31.4	-67.0
19, 23	$4.4e+04$	-44.3	-63.1	737	-40.0	-76.5
30, 32	$3.8e+04$	-56.8	-71.8	871	-47.0	-79.5
45, 46	$2.2e+05$	-59.0	-75.8	1758	-54.7	-96.1
48, 52	$1.7e+05$	-76.0	-93.8	2142	-58.1	-97.2

In general, since rational functions can use either real or complex poles to model the steep fluctuation present in given data, it is to be expected that the rational modeling technique gradually decides to locate its poles near the slopes of the given design. The model can also be made free of real poles in the domain of interest, while complex poles model the steepness present in that domain.

In Example 2, we model the transmission coefficient $S_{21}(f, w)$ of two perfectly conducting round posts centered in the E -plane of a rectangular waveguide. The diameter of the posts is set to 2 mm and the frequency f and post-spacing w vary over (7, 13 GHz) and (4, 18 mm), respectively. The problem is bivariate and complex valued, and the modulus and argument are modeled using the same datapoints. The results are displayed in Table IV and Fig. 3. We display the modulus and argument of both $S_{21}(f, w)$ and $r_{19,20}(f, w)$. We also display the true and estimated relative error in the modulus and argument. Let us point out that, as in the real-valued case, the datapoints are still selected on the basis of where $E_\ell(f, w)$ in (8) or, equivalently, $|R_\ell(f, w) - R_p(f, w)|/(1 + |R_\ell(f, w)|)$ attains a discrete maximum. Observe that $|r_{19,20}(f, w) - r_{16,22}(f, w)|/(1 + |r_{19,20}(f, w)|)$ is different from both the function plotted in Fig. 3(f) and Fig. 3(h). The gain in computing time is clear: with only 40 datapoints (for the computation of $r_{19,20}$) instead of 57 (a gain of 30%), a similar result is obtained. Since there are no poles of $r_{19,20}$ in the neighborhood of the interpolation space, we do not plot the denominator zeroes.

We next consider some trivariate problems. In Example 3, we model the reflection coefficient $S_{11}(f, h, \ell)$ of a capacitive step in a standard WR90 rectangular waveguide. The variables are the frequency f , the gap height h , and the step length ℓ . The interpolation space is chosen rather large to test the capabilities of the new method, namely, $7 \text{ GHz} \leq f \leq 13 \text{ GHz}$, $2 \text{ mm} \leq h \leq 8 \text{ mm}$, and $0.5 \text{ mm} \leq \ell \leq 5 \text{ mm}$. The results can be found in Table V. For this problem, a qualitatively comparable model can be realized with less than 5% of the datapoints used in [23]: 92 to reach at least -59-dB maximum error or 101 to obtain almost -94-dB mean error.

In Example 4, we model the trivariate transmission coefficient $S_{21}(f, a, b)$ of a 1-mm iris in a standard WR90 rectangular waveguide. The variables are the frequency $f \in [8, 12]$ in gigahertz, the gapwidth $a \in [8, 15]$ in millimeters, and the gap height $b \in [1, 3]$ in millimeters. The results are shown in Table VI. Now with less than 6% of the data required in [23], an equally accurate model ($\epsilon = -50 \text{ dB}$) can be constructed. In higher dimensions, the advantage of allowing the datapoints to be scattered in the interpolation space obviously pays off.

TABLE VI
IRIS IN RECTANGULAR WAVEGUIDE: TRANSMISSION COEFFICIENT

n, m	$\kappa_2(A)$	max	mean	S for [23]	max	mean
3, 9	$4.6e+02$	-20.6	-39.7	168	-18.0	-50.0
11, 14	$6.5e+03$	-38.4	-56.3	247	-19.5	-56.9
17, 15	$1.4e+04$	-42.7	-63.4	328	-31.1	-63.2
19, 17	$3.8e+04$	-49.2	-67.3	560	-33.1	-66.5
21, 20	$3.7e+04$	-53.4	-72.4	736	-52.6	-72.7

The study of the proposed technique when the microwave structure exhibits resonant behavior is part of ongoing work. In view of the fact that the new technique can easily handle steep changes in the parameter domain, this investigation is expected to be successful. Together with the forthcoming work, a MATLAB toolbox for the computation of the rational interpolant in any higher dimension will be made available.

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