

Polynomial-Based Surrogate Modeling of Microwave Structures in Frequency Domain Exploiting the Multinomial Theorem

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Abstract — We propose a methodology for developing EM-based polynomial surrogate models exploiting the multinomial theorem. Our methodology is compared against four EM surrogate modeling techniques: response surface modeling, support vector machines, generalized regression neural networks, and Kriging. Results show that the proposed polynomial surrogate modeling approach has the best performance among these techniques when using a very small amount of learning base points. The proposed methodology is illustrated by developing a surrogate model for a T-slot PIFA antenna simulated on a commercially available 3D FEM simulator.

Index Terms — surrogate modeling, polynomial surrogates, multinomial theorem, EM-based design, PIFA antenna, FEM.

I. INTRODUCTION

In most practical cases, direct optimization of high-frequency structures using full-wave EM simulators is computationally expensive. A way to speed up the optimization process is by using surrogate models [1]. Some of the most popular approaches for functional EM surrogate models include response surface methodology (RSM), artificial neural networks (ANN), support vector machines (SVM) and Kriging.

RSM represents the relationship between the input parameters and the output responses by a second-order polynomial. The minimum number of function evaluations is equal to the number of unknowns in the polynomial equation [2,3]. ANNs can approximate arbitrary nonlinear input-output deterministic relationships by using the proper amount of training and testing data as well as a suitable complexity; their training is typically based on some optimization algorithm [4]. An interesting case of ANN that does not require an iterative training procedure is the generalized regression neural network (GRNN) [5]. GRNNs are fast learning and converge to the optimal regression surface as the number of samples become large [5]. SVMs can solve complex constrained quadratic optimization problems due to the utilization of kernel functions. Training of the SVMs is based on the principle of structural risk minimization, which results on a good trade-off between the complexity of the model and the generalization capability [6,7]. Finally, Kriging models are based on the distance between the input location to be predicted and the input locations already observed; their weights are chosen to minimize the prediction variance using the best linear unbiased estimator. As the number of function evaluations increases, the Kriging predictions accuracy also increases [8,9].

The proposed methodology in this paper represents the

relationship between the input parameters and the output responses at each simulated frequency point by using polynomial functions based on the multinomial theorem. The multinomial theorem allows us to expand any polynomial function raised to an arbitrary power, including all cross terms. Our methodology is not limited to a second-order polynomial function, like RSM. The order of the surrogate model is increased until generalization error deteriorates. The amount of learning base points is not determined by the number of unknowns in the system. A global minimum is achieved in closed form during the weighting factors calculation.

A similar approach for EM-based polynomial surrogate modeling is proposed in [10], [11]. Our approach differs from [10] in that redundant terms for the surrogate model are not created. It also differs from [10] and [11] in that: 1) weighting factors are calculated by assuming that lower-order surrogates are already available and fixed, or by calculating all weighting factors simultaneously for each surrogate model order, depending on the system conditioning, and 2) surrogate model order can be different for each simulated frequency point.

II. POLYNOMIAL SURROGATE MODELING FORMULATION

Let $\mathbf{R}_f \in \mathbb{R}^p$ denote a fine model response sampled at p frequency points, whose design variables are in $\mathbf{x} \in \mathbb{R}^n$. The fine model is treated as a multidimensional vector function, $\mathbf{R}_f(\mathbf{x}) : X_f \rightarrow \mathbb{R}^p$ whose domain is $X_f \subseteq \mathbb{R}^n$. Our purpose is to develop a surrogate model $\mathbf{R}_s(\mathbf{x}) : X_s \rightarrow \mathbb{R}^p$ that approximates $\mathbf{R}_f(\mathbf{x})$ within a region of interest $X_s \subseteq X_f$, around the reference design $\mathbf{x}^{(0)}$, with $\Delta\mathbf{x} \in \mathbb{R}^n$ representing the distance from a given point to the reference design, $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}^{(0)}$. For brevity, here we describe our formulation up to the third-order surrogate.

The first-order surrogate model at the k -th simulated frequency point is defined as

$$R_{sk}^{(0)}(\mathbf{x}) = R_{fk}(\mathbf{x}^{(0)}) + \mathbf{w}_k^{(1)T} \mathbf{q}^{(1)}(\Delta\mathbf{x}) \quad (1)$$

where $\mathbf{w}_k^{(1)} \in \mathbb{R}^n$ contains the corresponding surrogate model weighting factors and $\mathbf{q}^{(1)}(\Delta\mathbf{x}) \in \mathbb{R}^n$ is a multidimensional vector function that contains the first-order multinomial terms for $\Delta\mathbf{x}$. The scalar elements of $\mathbf{q}^{(1)}$ are given by

$$q^{(1)}(\Delta\mathbf{x}) = \Delta x_{\lambda_1} \text{ for } \lambda_1 = 1:n \quad (2)$$

Similarly, the third-order surrogate model at the k -th simulated frequency point is defined as

$$R_{sk}^{(3)}(\mathbf{x}) = R_{sk}^{(2)}(\mathbf{x}) + \mathbf{w}_k^{(3)T} \mathbf{q}^{(3)}(\Delta\mathbf{x}) \quad (3)$$

where $\mathbf{w}_k^{(3)} \in \mathbb{R}^{n(n+1)(n+2)/6}$ contains the corresponding weighting

factors and $\mathbf{q}^{(3)}(\Delta \mathbf{x}) \in \Re^{n(n+1)(n+2)/6}$ contains the third-order multinomial terms whose scalar elements are given by

$$\mathbf{q}^{(3)}(\Delta \mathbf{x}) = \Delta x_{\lambda_1} \Delta x_{\lambda_2} \Delta x_{\lambda_3} \quad (4)$$

for $\lambda_1 = 1:n$, $\lambda_2 = \lambda_1:n$ and $\lambda_3 = \lambda_2:n$.

III. TRAINING THE POLYNOMIAL SURROGATE MODELS

The size of the training region X_s is defined by a vector $\boldsymbol{\tau} \in \Re^n$ containing the maximum relative deviation for each design variable with respect to $\mathbf{x}^{(0)}$. To train the surrogate model, we use L learning base points within X_s , denoted as $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(L)}$. To measure the generalization error of the surrogate model, we use T testing base points. The surrogate model weighting factors can be calculated: a) by assuming that the lower-order surrogates are already calculated and their weighting factors are fixed, or b) by calculating all the weighting factors simultaneously for each surrogate model order.

A. Weighting Factor Calculation with Lower-Order Surrogates Fixed

For the third-order surrogate model, we want to match the fine model response and the corresponding surrogate model response at the j -th learning base point and k -th frequency,

$$R_{sk}^{(2)}(\mathbf{x}^{(j)}) + \mathbf{w}_k^{(3)\top} \mathbf{q}^{(3)}(\Delta \mathbf{x}^{(j)}) = R_{fk}(\mathbf{x}^{(j)}) \quad (5)$$

Applying (5) for $j = 1, \dots, L$, and assuming that the lower-order surrogates are already calculated, the third-order surrogate weighting factors can be calculated by solving for $\mathbf{w}_k^{(3)}$ the following system of linear equations

$$\mathbf{Q}^{(3)} \mathbf{w}_k^{(3)} = \Delta \mathbf{R}_k^{(3)} \text{ for } k = 1 \dots p \quad (6)$$

where $\mathbf{Q}^{(3)} \in \Re^{L \times n(n+1)(n+2)/6}$ and $\Delta \mathbf{R}_k^{(3)} \in \Re^L$ are defined as

$$\mathbf{Q}^{(3)} = \begin{bmatrix} \mathbf{q}^{(3)}(\Delta \mathbf{x}^{(1)})^\top \\ \mathbf{q}^{(3)}(\Delta \mathbf{x}^{(2)})^\top \\ \vdots \\ \mathbf{q}^{(3)}(\Delta \mathbf{x}^{(L)})^\top \end{bmatrix} \quad (7)$$

$$\Delta \mathbf{R}_k^{(3)} = \begin{bmatrix} R_{fk}(\mathbf{x}^{(1)}) - R_{sk}^{(2)}(\mathbf{x}^{(1)}) \\ \vdots \\ R_{fk}(\mathbf{x}^{(L)}) - R_{sk}^{(2)}(\mathbf{x}^{(L)}) \end{bmatrix} \quad (8)$$

B. Calculating All Weighting Factors Simultaneously for Each Surrogate Model Order

For the third-order surrogate model, we want to match the fine model response and the corresponding surrogate model response at the j -th learning base point and k -th frequency,

$$R_{sk}^{(0)}(\mathbf{x}^{(j)}) + \mathbf{w}_k^{(1)\top} \mathbf{q}^{(1)}(\Delta \mathbf{x}^{(j)}) + \mathbf{w}_k^{(2)\top} \mathbf{q}^{(2)}(\Delta \mathbf{x}^{(j)}) + \mathbf{w}_k^{(3)\top} \mathbf{q}^{(3)}(\Delta \mathbf{x}^{(j)}) = R_{fk}(\mathbf{x}^{(j)}) \quad (9)$$

Applying (9) for $j = 1, \dots, L$, the surrogate model weighting factors can be calculated by solving for $\mathbf{W}^{(3)}$ the following system of linear equations

$$\mathbf{Q}_{\text{All}}^{(3)} \mathbf{W}^{(3)} = \Delta \mathbf{R}_k \text{ for } k = 1 \dots p \quad (10)$$

where $\mathbf{Q}_{\text{All}}^{(3)} \in \Re^{L \times n(n+1)/2 + n(n+1)(n+2)/6}$ and $\mathbf{W}^{(3)} \in$

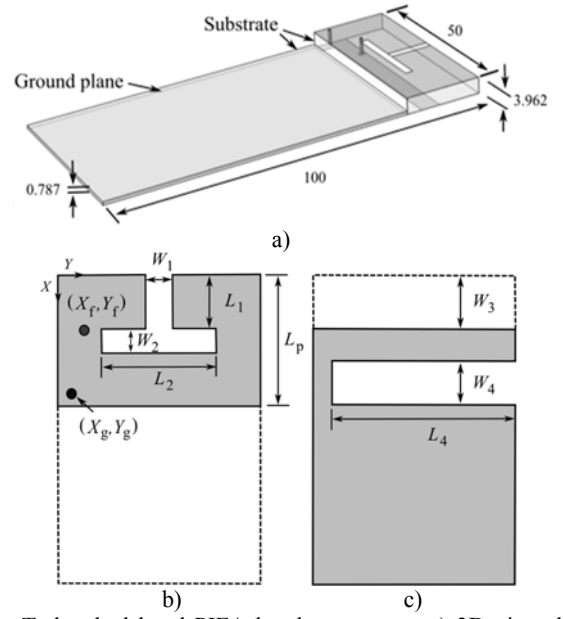


Fig. 1. T-slot dual band PIFA handset antenna: a) 3D view, b) top view, c) bottom view. From [12].

$\Re^{L \times n(n+1)/2 + n(n+1)(n+2)/6}$ are defined as

$$\mathbf{Q}_{\text{All}}^{(3)} = \begin{bmatrix} \mathbf{Q}^{(1)} & \mathbf{Q}^{(2)} & \mathbf{Q}^{(3)} \end{bmatrix} \quad (11)$$

$$\mathbf{W}^{(3)} = \begin{bmatrix} \mathbf{w}_k^{(1)} & \mathbf{w}_k^{(2)} & \mathbf{w}_k^{(3)} \end{bmatrix} \quad (12)$$

C. Automatic Selection of Best Conditioned System

Depending on the condition number of $\mathbf{Q}^{(3)}$ and $\mathbf{Q}_{\text{All}}^{(3)}$, we define how the weighting factors are calculated. If the condition number of $\mathbf{Q}^{(3)}$ is smaller than the condition number of $\mathbf{Q}_{\text{All}}^{(3)}$, weighting factors are obtained from (6), otherwise, from (10). This test is inexpensive (no fine model evaluations implied).

IV. EXAMPLE

Consider the T-slot dual band PIFA handset antenna [12] whose geometry is shown in Fig. 1. The T-slot in the patch is the main element of the antenna contributing to the dual-band resonances. The antenna is designed on a substrate with a relative permittivity $\epsilon_r = 2.2$, a dielectric loss tangent $\tan \delta = 0.009$ and a thickness $H = 3.962$ mm. The initial design parameters values are defined as $W_1 = 3.83$ mm, $W_2 = 8.85$ mm, $W_3 = 11$ mm, $W_4 = 1.54$ mm, $L_1 = 8.10$ mm, $L_2 = 20.34$ mm, $L_p = 24$ mm, $Y_f = 14$ mm, $X_f = 19.16$ mm, $Y_g = 18.9$ mm and, $X_g = 1$ mm. We implement the antenna structure in COMSOL.

We model the antenna return loss taking as input parameters $\mathbf{x} = [W_1 \ W_2 \ L_1 \ L_2]^\top$, on a reference design $\mathbf{x}^{(0)} = [3.83 \ 8.85 \ 8.10 \ 20.34]^\top$ (mm), over a region defined by $\boldsymbol{\tau} = [5\% \ 5\% \ 5\% \ 5\%]^\top$. EM response of the antenna at $\mathbf{x}^{(0)}$ is shown in Fig. 2.

We consider a very limited amount of learning base points, using a star ($2n$) and box distribution (2^n). Performance of the surrogate model is measured by calculating the maximum absolute error in the learning set at each frequency point,

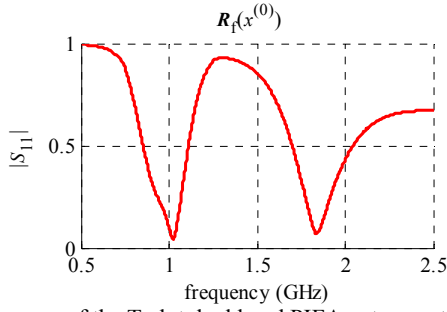


Fig. 2. Response of the T-slot dual band PIFA antenna at $x^{(0)}$.

denoted as ϵ_L , as well as in the testing set, denoted as ϵ_T . To denote the largest maximum absolute error in the complete frequency sweep we use ϵ_{Lmax} and ϵ_{Tmax} , for the learning and testing sets, respectively.

TABLE I

model	star distribution		box distribution	
	ϵ_{Tmax}	ϵ_{Lmax}	ϵ_{Tmax}	ϵ_{Lmax}
RSM	0.116770	0.080603	0.114430	0.107880
PSM	0.098251	0.054615	0.061406	0.013724
SVM	0.176450	0.077729	0.166740	0.166740
Kriging	0.106600	0.022197	0.066893	0.013126
GRNN	0.170990	0.081205	0.162690	0.162690

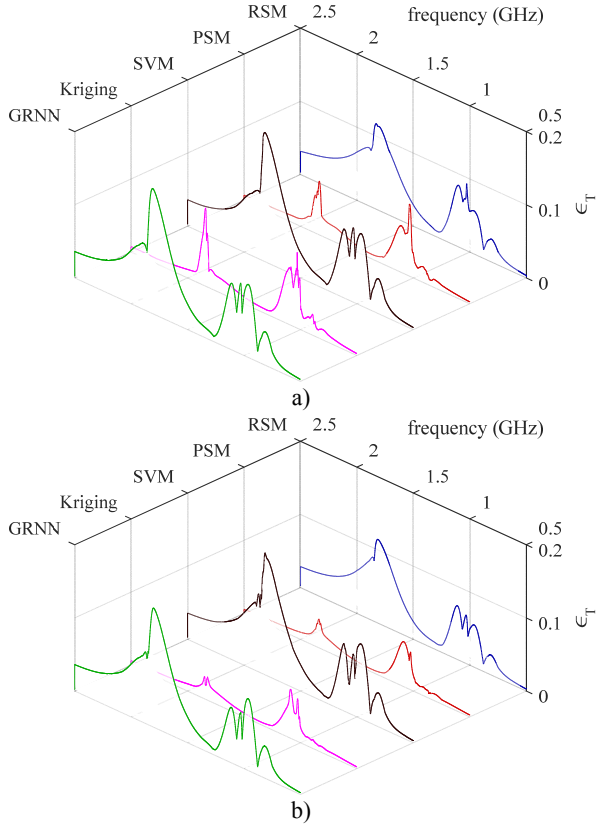


Fig. 3. Maximum testing errors for $|S_{11}|$ of the PIFA antenna using 81 uniformly distributed testing base points and: a) a star distribution of learning base points ($2n = 8$); b) a box distribution of learning base points ($2n = 16$).

The generalization performance of the proposed polynomial surrogate modeling (PSM) is compared against that one of the surrogate models based on RSM, SVM, Kriging, and GRNN. The corresponding results are shown in Table I and Fig. 3. It is seen that PSM exhibits the best generalization performance.

We have observed a similar performance for these modeling techniques in other two completely different microwave structures: the proposed PSM has the best performance when using a small amount of learning base points (star and box distributions). When using many learning base points, best performance among the five techniques varies depending on the structure. Details are omitted due to lack of space.

V. CONCLUSIONS

A new polynomial surrogate modeling (PSM) approach based on the multinomial theorem was presented. It calculates weighting factors using two different formulations, according to the best condition number of the system matrix. To improve generalization, polynomial order is different at each frequency. The proposed PSM proves to be suitable for surrogate modeling when the amount of learning base points is very limited.

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