Comparative Analysis of Approximation Methods in Electromagnetic Design

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Design optimization of complex electromagnetic devices such as antennas with volumetric material and conductor variations require high computational resources. This burden can be reduced by introducing cost-effective surrogate models into the design optimization framework. Here we present a comparative analysis of various surrogate modeling techniques for material design studies of electromagnetic devices. Also a new polynomial based approximation technique is proposed for modeling frequency based responses of complex electromagnetic devices especially exhibiting multi-resonance behavior.

I. Introduction

NUMERICAL simulation based design has evolved as an important design strategy in designing new electromagnetic devices. Large scale electromagnetic (EM) design optimization problems such as volumetric material explorations of antennas demand high computational resources. This is primarily a result of expensive frequency based simulations where the numerical analysis tool such as the Finite Element Analysis (FEA) is called upon at each frequency for each design alternative. Despite the fast development of computing power and technology, the computational cost of complex high-fidelity engineering analyses present itself as the major bottleneck. One approach to surpass this drawback is by introducing surrogate based modeling techniques into the iterative based design platform.1-2 Response surface techniques are used to model input and output relations of a given system to replace the conventional numerical analysis tool with a functional representation of the performance surface3,4. Response surface based EM design examples also include electromagnetic actuators5. Fast numerical methods are employed within electromagnetic modeling and simulation tools to achieve further speed-ups such as the integration of FE-BI6 method with kriging and divided rectangles (DIRECT) for EMC applications7. Lately, space mapping (SM) concepts are also introduced exploiting coarse model (usually in the form of computationally fast circuit-based model) alignment with a fine model (typically CPU intensive full-wave EM simulation)8. Another alternative to improve the computational efficiency of EM re-analysis is to use singular-value decomposition approach, which drastically reduces the order of the eigenvalue problem. By inspection of the singular values, the accuracy level of the procedure may be controlled. The technique is applied to the analysis of open and closed waveguides with arbitrary cross sections, lossy conductors, and anisotropic dielectric layers9. A framework where the surrogate model and simulator interact through a distributed environment, using established grid computing techniques thus decreasing model generation and simulation turnaround time2 was introduced as another speed-up technique.

Despite the large variety of techniques, some approximation schemes or surrogate modeling techniques will stand out in the literature such as polynomials, multiquadrics10, kriging and artificial neural networks (ANNs)11. The ‘virtual’ objective function they provide can be called by the optimization algorithm within a design cycle. Many Response Surface Methods such as space mapping techniques8 or combinations thereof are documented recently coupling especially the aforementioned approximation techniques with stochastic algorithms. Some methods are based on extrapolating local information12 while others are solution technique dependent such as Chebyshev interpolations applied to enhance the efficiency of the moment matching technique13. A comparative analysis of various surrogate models specifically for EM devices exhibiting multi-resonance behavior does not exist. Also, there are only few adaptive algorithms not requiring a-priori knowledge of the problem dynamics14. This paper provides a comparative study on various surrogate modeling techniques that could be used in the design of non-intuitive electromagnetic systems exhibiting multi-resonance behavior. Following the comparative study of four

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surrogate based methods, namely, Artificial Neural Networks (ANN), Radial Basis Functions (RBF), Support Vector Machines (SVM) and kriging. A polynomial based approximation technique is proposed for modeling multi-resonance based frequency response of complex electromagnetic devices. Based on the results of the comparative study, ANN and RBF are more convenient surrogate modeling techniques for design spaces including resonances considering surface quality and model construction time. The proposed polynomial based approximation method here is capable of reducing the number of FEM calls during an optimization process significantly. Despite the multi-resonance characteristics of the return loss response, the method is capable of fitting good quality rational functions between adaptively selected support points (i.e. frequency points) without a-priori system knowledge.

II. Overview of Approximation Methods

Several factors exist in choosing the most appropriate surrogate model. These include the complexity and functional characteristics of the analysis model to be replaced and the effort in determining the surrogate model. In this study we first compare the performance of different surrogate models in approximating the frequency response of electromagnetic devices to make that choice easier for similar design optimization studies. Most popular surrogate models include polynomials, Radial Basis Functions (RBF), Kriging, Neural Networks and Support Vector Machines (SVM) and are studied here.

Polynomial models, seem to be one of the natural choices for resonance based surrogate-modeling of electromagnetic devices since transfer functions of EM devices can in principle be represented by a rational function in the frequency domain. Polynomial models are fairly easy to implement, clear on parameter sensitivity, and cheap to work with but are usually less accurate than the Kriging model. However, polynomial functions do not interpolate between sample points directly and are limited by the chosen function type unless the function type is adaptively chosen. Similarly, RBF methods are very popular for scattered data interpolation. They try to approximate available data by a linear combination of translates of a single basis function. The main advantage, compared to polynomial models, is that they can handle vast amount of data points. On the other hand, computations involving RBF quickly become infeasible as the dimension of the input space increases. Unlike rational functions they lack a theoretical connection with the physical problem at hand, so one would expect less favorable results when using RBF for surrogate modeling. Similarly, the RBF based surrogate models especially the multi-quadric RBFs are easy to construct and can interpolate sample points at the same time. RBF is advantageous since it results in a linear problem that is non-singular, proving RBFs especially useful in the model construction where multi-parametric models are involved. Regarding Kriging, more accurate models especially for nonlinear problems are usually obtained but these models are difficult to obtain and to use. Most of the time, global optimization is needed to identify their maximum likelihood estimators. Kriging is also flexible in either fitting or filtering noisy data. Successful implementations exist in literature for a limited number of design variables. Neural networks, on the other hand, are widely used in the field of statistics to automatically build models describing complex relations between input and output with a low computational cost. The basic principle of neural networks is to create an approximation of a complex function by combining simple elementary functions. In addition, it is known that Kriging and RBF are both more sensitive to numerical noise than polynomial models. Finally, support vector machines (SVMs) are a set of related supervised learning methods used for classification and regression. They belong to a family of generalized linear classifiers. A special property of SVMs is that they simultaneously minimize the empirical classification error and maximize the geometric margin; hence they are also known as maximum margin classifiers.

In the second half of this study, to overcome challenges in fitting multi-resonance based electromagnetic behavior and to allow for further speed-ups, a new rational function approximation model based on a modified Bulirsch and Stoer (BST) recursive interpolation technique is proposed. Polynomial models seem to be one of the natural choices for resonance based surrogate-modelling of electromagnetic devices since transfer functions of EM devices can in principle be represented by a rational function in the frequency domain. The recursive behavior proposed here improves its applicability to adaptive sampling schemes. When compared with direct matrix solutions of the rational interpolation, BST is significantly less prone to numerical errors and is not constrained by the rank of the system. Our proposed technique is based on a modified BST approach not necessarily following the diagonal Neville path in a conventional BST. This is expected to result in increased degrees of freedom for selecting the next support point and to enhance the reliability of the adaptive fitting technique.
III. Generation of Approximate Models

The primary objective here is to compare various surrogate modeling methods for their suitability for existing material based design optimization frameworks for electromagnetic applications. The comparative study is the major focus of this paper and should provide a best surrogate based models candidate to be integrated with suitable design optimization techniques towards the ultimate goal of designing volumetric material and conductor variations of complex electromagnetic devices. Analysis modules for constructing the surrogate models in the comparative study correspond to a commercial full wave electromagnetic solver, Ansoft HFSS. An in-house hybrid full-wave FE-BI based analysis tool is used for approximating multi-resonance behavior via modified BST algorithm. The surrogate model generation framework is primarily based on interfacing the analysis tools with various surrogate based models and with a MATLAB based Graphical User Interface.

The surrogate model framework is constructed for the return loss response of a patch antenna shown in Fig. 1. The chosen surrogate model can be linked to various optimization techniques to design RF devices such as patch antennas subject to bandwidth and miniaturization requirements. A standard problem could address to determine optimal values of the permittivity and permeability of the magneto-dielectric substrate(s) of possibly a multi-substrate layer probe fed antenna. The antenna chosen here is analyzed via FEA based analysis tools to compute its frequency based return loss ($s_{11}$) response. Substrate permittivity and permeability values here are chosen to vary between 1-16. A suitable objective function to maximize bandwidth is $f(x) = \min[max(|s_{11}|_i)]$ where $i = 1,...,N_{freq}$ represents frequency index of $N_{freq}$ number of discrete frequency points sampled within the chosen frequency range of operation of 1-2.5 GHz and $x$ is the design vector such as the permittivity of the dielectric substrate. The size of the design space could increase depending on the number of substrate layers of the system. The variables chosen here correspond to the dielectric permittivity and the frequency of operation of the antenna for a single layer substrate patch antenna. A standard FEA based optimization search via SQP would require 2 runs per design variable for each frequency data at each iteration. With a single full wave analysis taking about 300-900 seconds this search will become computationally impractical with increasing number of design variables (such as multi-material and conductor properties) and infeasible via global search algorithms such as the Genetic Algorithm. Here we investigate specific surrogate modeling techniques for approximating the antenna performance to speed-up materials based antenna design efforts exhibiting resonance behavior.

To investigate the performance of aforementioned surrogate models on the same design problem, these techniques are applied to approximate the return loss response of a simple patch antenna with one magneto-dielectric substrate. The desired performance of the surrogate model is to capture the resonance behavior with as less sample data as possible thus reducing the overall computational cost of the approximate model. This approximate model is going to replace the FEA based HFSS model in repetitive analysis calls when calculating the bandwidth in a general design optimization problem described earlier. To allow for considerable speed-ups in such design efforts, an adaptive Design of Experiment (DOE) scheme is integrated in an automated fashion to each surrogate modeling tool. Four different models are tested within the same framework: Artificial Neural Networks (ANN), RBF (Radial Basis Functions), Support Vector Machines (SVM) and Kriging. Each surrogate model is constructed based on the outputs of the EM simulator for a limited number of intelligently chosen data points. More specifically, surrogate models are created by integrating a commercial high frequency analysis tool, Ansoft HFSS with a MATLAB programming environment to automate the experiments a DOE scheme requires. HFSS simulates the exact electromagnetic response of the device and the Latin Hypercube Method is used as the Design of Experiments (DOE) scheme. It systematically investigates the system where a series of structured tests are designed in which planned changes are made to the input variables of the system. To generate surrogate models, Surrogate Modeling Toolbox (SUMO) is integrated with our automated DOE platform. In addition to the DOE scheme, adaptive sampling based on the hybridization of the accuracy of the model and density of the samples is used with the objective of producing models with improved quality for models provided by SUMO. As a model validation metric, validation set (%80 of sampling for training, %20 of sampling for validation) is used. The error measure is defined as the root relative square error (RLSE) which is defined by Eq. (1) as follows:

$$ \text{RLSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{y_i - \hat{y}_i}{y_i} \right)^2} $$
\[ E = \sqrt{\frac{\text{MSE}}{\text{Varience}}} \]  

where MSE is the Mean Square Error. Error measure is set to 0.1 in constructing the models.

After the comparative study, to explore the possibility of fitting multi-resonance based electromagnetic behavior of more complex electromagnetic structures rational function based polynomial fittings are also investigated. Multi-resonance behavior is encountered within the global design search of antennas of various shapes printed on multi-material magneto-dielectric substrates. The goal similar to the comparative study is to use the resulting approximate model to predict antenna performance when designing for enhanced antenna performance such as large bandwidth and small size. Solving for the appropriate rational model satisfying support point conditions is a challenging task due to the resulting ill-conditioned system of equations. The linear system solution becomes more prone to numerical error as the number of support points increases. Solutions to this problem exist which are mostly data sensitive especially as the number of support points increases, require extensive memory storage and the system needs to be resolved for each additional point. An alternative solution is presented via a recursive technique initially introduced by Stoer and Bulirsch (BST). The recursive behavior enhances its applicability to adaptive sampling techniques. When compared with direct matrix solutions of the rational interpolation, BST is significantly less prone to numerical errors and is not constrained by the rank of the system. Our proposed technique is based on a modified BST approach not necessarily following the diagonal Neville path in a conventional BST. This is expected to result in increased degrees of freedom for selecting the next support point and to enhance the reliability of the adaptive fitting technique. Adaptive sampling using conventional BST is usually determined at the maximum error norm of two successive curve fitting interpolators and follows the diagonal Neville path to construct the resulting interpolating function with at most one order difference between the numerator and the denominator. Our approach relies on expanding the solution freedom to an arbitrary Neville path, that allows for higher order differences and hence, more freedom in choosing more informative support points. As a result, improved convergence behavior is expected by preventing premature convergence and reducing the iteration numbers to reach faster global convergence when compared to conventional BST. The normalized error threshold of two successive interpolators is chosen to be 4 dB/db in this study.

The interpolated data in this part relates to the response of an antenna model similar to Fig. 1 that comprises a geometry discretized by 400 volumetric/layer and 400 surface finite elements. Properties such as permittivity, permeability and conductivity of each Finite Element cell of each layer could be assigned as design variables in a large-scale design problem. The use of global design search efforts to optimize the device and locate the global optimum will call for multiple reanalysis of the full-wave bandwidth response. In order to predict the return loss response accurately, a rather ‘fine’ frequency sampling (10 MHz for the antenna in Fig. 1) is needed. Spatially variable magneto-dielectrics and conductors may result in high oscillations/multiple resonances within the frequency range of interest. This makes the efficient prediction of the response an extremely challenging task. In the proposed adaptive sampling strategy data is always sampled at the frequency with the maximum error between two successive interpolators that pass through enough support points of the corresponding iterations.

### IV. Results

Several surrogate models are investigated with respect to their performance in capturing the return loss response of a resonance patch antenna with respect to varying frequency of operation and substrate dielectric constant. For all surrogate models, the type of DOE, sampling method, error norm and hyperparameter Genetic optimization algorithm which is used to optimize model based parameters, are the same.

Results of the ANN based surrogate model is shown in Fig. 2. User specified model parameters comprise a three layered MLP structure and 300 epochs. Initial weights are chosen to be in a range of [-0.8 - 0.8]. As transfer functions, both hyperbolic tangent sigmoid and linear transfer functions are used. Genetic algorithms are used for optimizing the weights to minimize the model error. As learning rules, bayesian regulation backpropagation, Levenberg-Marquardt backpropagation and scaled conjugate gradient backpropagation are used. The model converged to the response in Fig. 2 after collecting 345 samples using an adaptive DOE strategy.
As a second surrogate model, Radial Basis Functions are investigated with an emphasis on the following basis functions: Gaussian, multiquadric and exponential. The variable ranges for the functions are [0.1-5] in logarithmic scale. Regressions values are chosen to be [-1,0,1,2]. Within this setting, the RBF Model converged to the return loss response in Fig. 2.b with a model error norm of 0.1 after collecting 274 samples with an adaptive DOE. Results are satisfactory in terms of capturing resonance even as the dielectric constant increases. Also model construction requires less sample data than the ANN-based model in Figure 2.a. However, it is noted that RBF is observed to be more sensitive to sample distribution.

For the 3rd model via SVM, user specified parameters comprise the Kernel Parameter bounds chosen to be [-4, 4] and Regression Parameter bounds to be [-5,5]. SVM based model converged to the response surface plotted in Fig. 2.c. With overall 344 sample data it is slower than the RBF based model construction but faster than the ANN based model. It is also observed that it is less sensitive to sample distributions when compared to kriging. The model mimics clearly the shifted resonance response of the return loss with 344 samples. However, it is not as successful as ANN and RBF based models considering its non-smooth characteristics of its resulting response surface.

Figure 2. Surrogate modeling results
As the final model, to construct a Kriging based model for the return loss response correlation function alternatives such as spline, exponential, linear and Gaussian exist. Gaussian correlation is chosen for this study based on preliminary testing of similar resonance based response functions. For the correlation parameter, theta, lower bound is chosen as -5 and upper bound is chosen 3. First order Polynomial regression is performed next. Model hyper-parameters are found by a genetic algorithm. The response surface is able to capture the resonance of the patch antenna with 164 sample data as shown in Fig. 2 d.

Interpolation results for a patch antenna return loss response versus frequency using adaptive sampling with a modified Neville Path Burlisch-Stoer algorithm is shown in Fig. 3. The interpolation result is compared to the original response curve numerically calculated using a fine sampling rate of 10 MHz, i.e. 101 uniformly distributed frequency points are sampled between 1-2 GHz to construct the return loss response. Since finer sampling does not improve the response further, it is accepted as the original antenna response. As shown in Fig. 3, results adopting the proposed technique based on the adaptive Neville path show that all resonances < -1dB are successfully captured.

![Graph](image)

\textbf{Figure 3.} Return loss response vs. frequency (Adaptive BST algorithm (red) vs. actual response (blue) and linear interpolation (dashed line)).

With 29 adaptively sampled data points shown in triangular legend shapes in Fig.3 vs. 101 uniformly sampled data points originally needed, significant reduction in computational time was achieved. Specifically, the proposed algorithm reduced the number of simulations by a factor of 3. The speed-up algorithms could be adapted to large scale design optimization studies which comprise a future work topic.

\section{V. Conclusion}

Several surrogate modeling techniques such as ANN, RBF, SVM and Kriging are analyzed comparatively to construct the frequency based return loss response of a dielectric substrate supported microstrip patch antenna. Also a polynomial approximation technique suitable for multi-resonance electromagnetic response behavior is proposed. Results based on investigations so far show that ANN and RBF are more promising in terms of capturing the overall resonance behavior of the patch antenna when compared with Kriging and SVM. Overall ANN is suggested to be used in surrogate model assisted material based design optimization studies for such antennas and can be analyzed further for increased number of model variables. Also, results show that the proposed rational model based recursive model is successful in fitting highly resonant antenna structures. Results suggest that an ANN based surrogate model design framework if integrated to the rational model based BST algorithm proposed here could allow for effective global explorations of the large scale design space when designing novel electromagnetic devices with multi-material substrates.
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