Gradient Based Reverse ANN Modeling Approach for RF/Microwave Computer Aided Design

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Abstract—**In this work, a new gradient based reverse modeling approach employing Artificial Neural Networks (ANNs) for systematic RF/microwave modeling is introduced. This approach is particularly suited to modeling scenarios, where standard ANN multi-layer perceptron (MLP) fails to deliver a satisfactory model. The proposed approach detects the simplest input-output relationship inherent to the modeling problem, which we term as the reverse model as compared to the original model (i.e., the modeling problem using standard ANN model). This reverse model is short-listed from a pool of candidate models obtained by systematically reversing the input-output variables of the original modeling problem, while retaining the ANN's structural simplicity. The proposed reverse and the not-so-accurate original models complement each other to yield accurate models. The advantages of this approach are demonstrated *via* modeling transmission lines and spiral inductors.**

Keywords-ANN; conjugate gradient; modeling; optimization; reverse model; sensitivity; spiral inductor; transmission line

I. INTRODUCTION

Artificial Neural Networks (ANNs) are one of the most popular modeling function approximation methods that continue to gain tremendous attention in the RF/microwave domain [1]–[4]. ANNs learn component behavior from full-wave electromagnetic (EM) simulations and/or measurements *via* a training process involving weight optimization [5]. In scenarios where conventional or standard ANN (e.g., Multi-Layer Perceptrons or MLP) fail due to complexities in the modeling problem (e.g., highly nonlinear RF/microwave input-output scenarios), the practice is to opt for new/sophisticated ANN architectures [6]. Such structures include Knowledge Based Neural Networks (KBNNs) that have been shown to model highly complicated RF/microwave data with improved extrapolation capabilities [7]. A prerequisite to knowledge architectures is the existence of prior knowledge e.g., empirical models or equivalent circuits, which may not always be available for new components [7, 8]. In [9], neural nets and fuzzy rules were combined. However, such approaches lead to increased complexity in model structure.

This research explores new approaches to ANN modeling that deal with complicated modeling problems while retaining structural simplicity. The proposed approach advocates an intermediary model termed as "reverse model" with a different structure that is accurate relative to the desired or original model. The accurate reverse model and the not-so-accurate original model form a synergetic pair which turns out to be an accurate model for the original problem. In terms of implementation, the proposed approach mandates a root-finding algorithm (or an optimization routine). To this end, we employ three different candidates: (i) Sensitivity technique; (ii) Conjugate Gradient (CG); and (iii) Fletcher Reeves Conjugate Gradient (FRCG). The robustness of the proposed approach is illustrated through RF modeling examples.

II. PROPOSED MODEL DEVELOPMENT PHASE

Consider x as an n-vector containing inputs and y as an m-vector containing outputs of an RF/microwave modeling problem where the relationship between x and y is given by $y = f(x)$. For concept illustration in this initial study, we considered models with only one output. However, this approach can be extended for multiple outputs. Typically, data from electromagnetic (EM) simulators and/or measurements is used to develop an ANN model $y = f_{ann}(x, w)$, where w is the weight vector. An error/quality measure E is defined as

$$E = \sqrt{\frac{1}{P}\sum_{i=1}^{p}\left(\frac{y^i - f_{ann}(x^i, w)}{y^i}\right)} \times 100 \cdot \quad (1)$$

In (1), p denotes number of training data (x^i, y^i), where y^i is desired output and $f_{ann}(x^i, w)$ is ANN output when input is x^i. When the standard ANN model (e.g., MLP) fails to achieve user-defined quality (i.e., $E > E_{user}$ after exhaustive re-training) and KBNN is not feasible (i.e., there exists no knowledge or KBNN is human intensive), we advocate the proposed reverse modeling approach. In the proposed approach, a set of "candidate reverse models" is identified, by swapping the only output of the desired model with one input at a time. Suppose a desired/original modeling problem given by

$$y = f_{ann}(x_1, x_2, x_3, ..., x_n, w) \cdot \quad (2)$$

As such, the pool of candidate reverse models turns out to be:

$$x_{1,c} = f_{ann,1}(y, x_2, x_3, ..., x_n, w_1)$$
$$x_{2,c} = f_{ann,2}(x_1, y, x_3, ..., x_n, w_2)$$
$$\cdot$$
$$\cdot \quad (3)$$
$$\cdot$$
$$x_{n,c} = f_{ann,2}(x_1, x_2, ..., x_{n-1}, y, w_n),$$

where $f_{ann,i}$ denotes the ith candidate reverse model, $i \in [1, n]$, $x_{i,c}$ is the output of the ith candidate reverse model, and w_i denotes corresponding weight vector. In (3), it is clear that outputs of reverse models are inputs of the desired/original model. This approach mandates computer-aided training of candidate reverse models; however, such training requires no additional EM data. Data for training reverse models is simply obtained by swapping the corresponding input and output data columns. Once the full set of candidate reverse models is developed, we select the reverse model, based on quality measure E. The summary of the procedure follows: First, the candidate reverse model $f_{ann,1}$ is trained using rearranged training data. Given a rearranged input sample to $f_{ann,1}$ leads to estimation of output $x_{1,c}$ (an approximation of x_1). Second, error measure E_1 is evaluated. This procedure is repeated n times resulting in error measures E_1, E_2..., and E_n. The reverse model $f_{ann,j}$ with the least error is selected according to

$$j = \arg[\min_i E_i] . \qquad (4)$$

For a given input vector x, RF/microwave output/response y can be computed using: (i) the not-so-accurate desired/original model f_{ann}; (ii) the reverse model $f_{ann,j}$; and (iii) a typical root-finding algorithm. Details are provided in the following section.

III. PROPOSED MODEL UTILIZATION PHASE

The earlier section highlights model development process, while this section emphasizes model utilization. Given any input x, the objective is to accurately estimate y, by employing both f_{ann} and $f_{ann,j}$ in a collaborative way (see the pseudo-code). For a given x, the not-so-accurate desired/original model f_{ann} helps initialize the desired output y. Relevant inputs including this initial estimate are then fed to the relatively accurate correction model (i.e., $f_{ann,j}$ the reverse model). From this point forward, y is iteratively adjusted, until output of the correction model $f_{ann,j}$, converges to the given/known value x_j. Such iterations involve typical optimization routine(s) providing both updated direction and value of y. As mentioned earlier, three optimization techniques, (i) Sensitivity; (ii) CG; and (iii) FRCG, are implemented and their performances are compared through examples.

In the Sensitivity technique, partial derivatives (or the Jacobian) of the reverse model $f_{ann,j}$ with respect to y is computed using chain rule of calculus. The ratio of the residue to the Jacobian becomes the update value. In the Fletcher-Reeves CG method, each iteration involves the computation of update direction of conjugate p_k, gradient g_k, and α_k [10]. Learning rate α_k is chosen to minimize the error measure E in (1). In this research work, Golden-Section technique is implemented to find the optimal learning rate. For the benefit of the readers, we present the Golden-section method. Set $\alpha_1 > 0$ and $\alpha_2 < 1$, thus
- Compute $E(\alpha_1)$ and $E(\alpha_2)$
- If $E(\alpha_1) < E(\alpha_2)$, then set $\alpha_2 = \alpha_1 - 0.618(\alpha_1 - \alpha_2)$
- If $E(\alpha_1) > E(\alpha_2)$, then set $\alpha_2 = \alpha_1 + 0.618(\alpha_1 - \alpha_2)$
- Repeat this process until $(\alpha_1 - \alpha_2) < \varepsilon$.

where $E(\alpha) = E(y_k + \alpha p_k)$ and 0.618 is called Golden Mean or Golden Section. CG method is similar to Fletcher-Reeves CG except that α_k is obtained from residue instead of line search

and g_k is simply replaced by the residue. In this work, we present the pseudo-code involving FRCG method alone since steps 1 through 4 of pseudo-code remain the same for CG and Sensitivity techniques. Only step 5, the process of updating y, varies with the method as mentioned above.

Pseudo-Code of the Model Utilization Phase (FRCG Case)

Step 1: Given x, initialize y using the not-so-accurate desired/ original model f_{ann} developed using the conventional/standard ANN approach;

Step 2: Feed inputs $(x_1, x_2, x_3, ..., x_{j-1}, y, x_{j+1}, ..., x_n)$ to the proposed reverse model $f_{ann,j}$ to compute $x_{j,c}$, which is an approximate of x_j;

Step 3: Evaluate the objective function E_{obj} according to (1);

Step 4: Set $p_0 = -g_0$ (i.e., Sensitivity data from reverse model $f_{ann,j}$) and $y_0 =$ output of the not-so-accurate standard ANN/MLP model;

Step 5: If $|E_{obj}| \leq E_{user}$, RETURN y_0 and GOTO Step 6.

Else {   Compute α_k;

$\qquad y_{k+1} = y_k + \alpha_k p_k$;

$\qquad$ Evaluate gradient g_{k+1}; (Sensitivity data from $f_{ann,j}$)

$\qquad \beta_{k+1} = \dfrac{g_{k+1}^{T} g_{k+1}}{g_k^{T} g_k}$;

$\qquad p_{k+1} = -g_k + \beta_{k+1} p_k$;

$\qquad k = k+1$;

};

Step 6: STOP

IV. ILLUSTRATIVE EXAMPLES

The usefullness of the proposed approach includes diverse RF/Microwave components in the design stage (e.g., Microwave antennas, filters, etc.) where the geometrical dimension is employed as an output and S-parameters as inputs (i.e., given by the design specs) for practical implementations. Now two examples are introduced for demonstrating the robustness of the proposed approach.

A. Transmission Line Modeling

This example involves using the proposed technique to model a metal-insulator-semiconductor transmission line. It is of immense interest to employ ANN models for rapid structural optimization of the line geometry to obtain desired RF responses. We define desired/original ANN model as

$$W = f_{ann}(L, T, |S_{11}|, w), \qquad (5)$$

where W denotes line width, L denotes line length, T denotes oxide thickness, S_{11} denotes the reflection coefficient, and w is the adjustable weight vector of the MLP network f_{ann}. This model will provide useful information for designers to find a transmission line that matches the design specification. Training data is obtained using Sonnet EM[1] by varying the parameters of the transmission line: L (from 10 to 3000 μm), W (from 5 to 80 μm), T (from 0.25 to 2 μm), and frequency (from 0.1 to 12 GHz), resulting in 16,200 S-parameter simulation data. Data is randomized and 14,580 data is employed for training a standard ANN and 1,620 for verification. Quality measure E of the standard ANN turned out to be an unacceptable and equals to10.70%.

Therefore, the proposed approach is applied. First, the four candidate reverse models $f_{ann,1}$, $f_{ann,2}$, $f_{ann,3}$, and $f_{ann,4}$ are trained using 14,580 data. E for these models is 16.64%, 13.63%, 15.32%, and 4.80% respectively. Based on (4), $f_{ann,4}$ with output $|S_{11}|$ emerged as the reverse model. This concludes model development phase and model utilization phase begins. Given a new input vector x, accurate model output y can be rapidly computed *via* pseudo-code. Table I presents model errors for the entire data set including the training data (i.e., 16,200 samples) for the proposed reverse modeling approach based on all three root-finding techniques. To make the figures simpler 50 randomly selected data are used for comparing the line width (W) estimation from the proposed reverse ANN model with that from EM simulations. For simplicity, Fig. 1 only presents EM simulations *versus* FRCG and Sensitivity techniques but not the CG technique. It is clearly seen that the EM simulation results are well matched with that of FRCG technique. Error comparison of three optimization routines is presented in Fig. 2. FRCG technique illustrates major improvement over the conventional straightforward ANN approach (see Transmission Line example in Table I).
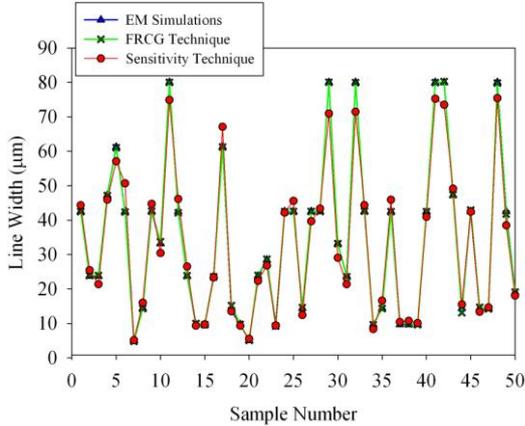

Figure 1.   Comparison of outputs from EM simulations versus FRCG and Sensitivity techniques for transmission line example.
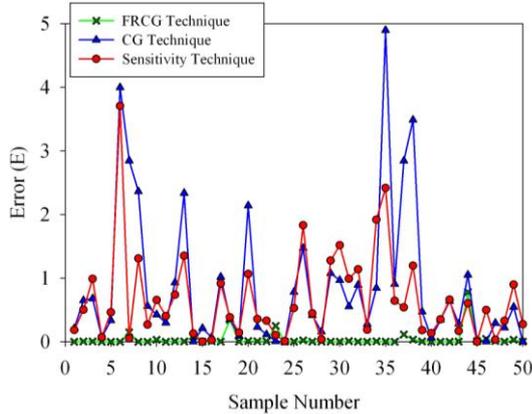

Figure 2.   Comparison of errors from FRCG, CG and Sensitivity techniques for transmission line example.

B.   Spiral Inductor Modeling

Despite its concise structure, optimization of spiral inductor is a complicated task [11]. Desired/original modeling problem employing an ANN is given by

$$d_{in} = f_{ann}(N, W, |S_{11}|, w), \qquad (6)$$

where d_{in} denotes inner diameter, N denotes number of turns, W denotes line width, S_{11} denotes the reflection coefficient, and w denotes ANN weights. Here, the inductance of an inductor can be calculated through S_{11}.
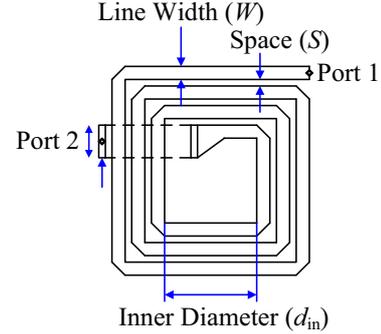

Figure 3.   Top-view of the spiral inductor.

Training data for the spiral inductor (Fig. 3) is obtained *via* Sonnet EM simulation fixing outer diameter at 250 μm and varying N (from 1 to 5), W (from 5 to 10 μm), frequency (from 0.25 to 12 GHz), and d_{in} (from 26 to 250 μm) resulting in a total of 3,304 S-parameter data. Quality measure E of the standard ANN model turned out to be unacceptable and equals to 12.02%. The proposed approach is applied and four candidate reverse models are developed by swapping the output (i.e., d_{in}) with one input at a time. According to (4), $f_{ann,4}$ with output $|S_{11}|$ emerged as "the reverse model" with $E = 6.31\%$. Following the model development, for any given input x, the proposed ANN model output can be computed using the pseudo code. The error percentages are presented in Table I. Comparison between EM data and the proposed approach based on Sensitivity and FRCG techniques is shown in Fig. 4. It is clearly observed that the EM simulation results are well agreed with that of FRCG technique. The accuracy of the three optimization routines is presented in Fig. 5. Of the three, the FRCG technique offers highest accuracies to the proposed reverse ANN approach.

TABLE I.   COMPARISON OF MODEL ERRORS FOR EXAMPLES A&B

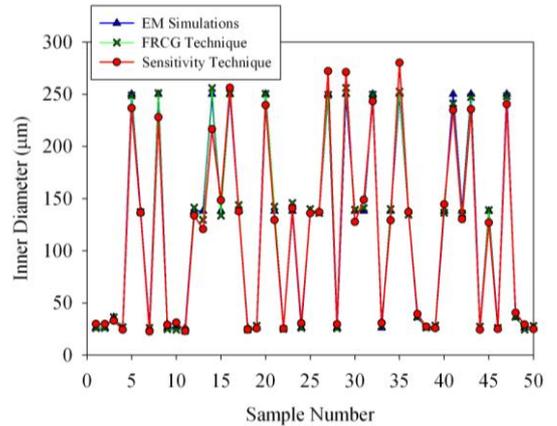| Example	Standard MLP	FRCG	CG	Sensitivity Technique
Transmission Line	10.70%	1.04%	5.81%	4.18%
Spiral Inductor	12.02%	2.51%	7.40%	5.89%

Figure 4.   Comparison of outputs from EM simulations versus FRCG and Sensitivity techniques for spiral inductor example.
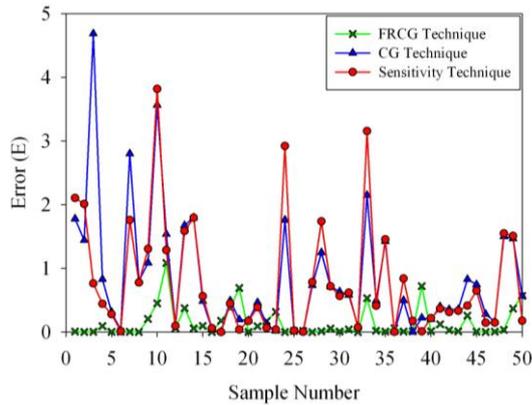
Figure 5. Comparison of errors from CG, Sensitivity and FRCG techniques for spiral inductor example.

TABLE II.   TIME COMPARISON OF THREE OPTIMIZATION ROUTINES

Example	Sensitivity Approach	CG	FRCG
Transmission Line	243.16s	430.42s	212.5s
Spiral Inductor	57.89s	81.74s	42.27s

In general, the elapsed time for data generation using EM solvers is computationally intensive. Using the proposed approach, the computational time can be alleviated. Comparison of elapsed time for model utilization phase of reverse models for entire data set (i.e., 16,200 samples for Transmission Line and 3,340 samples for Spiral Inductor examples) based on three optimization routines is presented in Table II. The elapsed time per sample is presented in Fig. 6. As can be seen, FRCG technique led to faster convergence. Tests are performed on a PC running on Intel Core™2 Duo E8600.
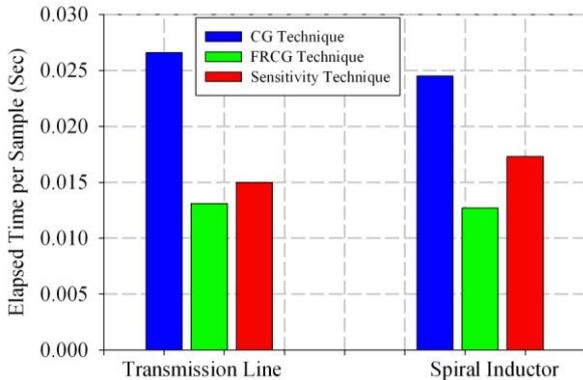

Figure 6. Elapsed time per sample of CG, FRCG and sensitivity techniques for both eamples A&B.

The reverse-modeling approach offers an effective solution for handling over-extended computational requirements in RF/microwave field. Implementation of this approach will require generation of data using full-wave EM solvers and/or high-frequency measurements by varying design parameters, which could be time-consuming. However, it is to be noted that as in other approaches (e.g., conventional ANNs and support vector machines), once data is ready, model development is computer-driven. In the modeling cases where standard ANN fails to deliver satisfactory results, the reverse-modeling approach is a simpler alternative to knowledge based modeling approaches. In terms of human or manual effort, the original data file simply needs to be rearranged per the structure of the candidate reverse-models (i.e., mere swapping of columns in the data file).

Output of the less accurate desired model is used as the initial guess in the proposed pseudo code. As such, the error between EM/physics simulations and the estimated value from standard ANN model is small resulting in faster rate of convergence. The advantage with conjugate gradient and its derived techniques lies in the property of conjugacy which notifies that the minimax function can be optimized in fixed number of steps.

V.   CONCLUSION

For the first time, this paper introduced a gradient-based reverse ANN modeling approach for efficient CAD modeling applicable in RF/microwave context. In a situation where standard MLP network fails and KBNN-type network is not an alternative, the proposed approach offers an accurate/fast model with its structural simplicity duly preserved. Initializing root-search with the empirical model (i.e., the straightforward ANN model) offers reasonable trust in terms of convergence. Being the first study in this direction, the proposed approach covers modeling cases with only one output. The extension to multiple outputs becomes a natural progression for future work. It is believed that this university-industry joint research is of practical interest to RF/microwave CAD community.

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