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End-to-end inverse modeling and optimization for filters based on artificial neural network

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Abstract

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INTRODUCTION 1

The designs of most passive microwave components, such as splitters, filters, and antennas, usually involve physical structures and corresponding electromagnetic (EM) responses. To design a filter with desired EM responses, structural parameter sweeps in full-wave EM simulations are essential, but these are time-consuming and labor-intensive. In recent years, with the improvement of computing power and the development of artificial intelligence, more and more work has applied neural networks to the design of microwave filters.^{1,2} Due to their excellent generalization ability when characterizing non-linear and non-analytic relations, artificial neural networks (ANNs) have been used as the surrogate model and are much faster than EM simulations. When combined with optimization algorithms, the surrogate model

local optima. This method is applied to designs of fourth-order interdigital cavity filters. The measurement and simulation agree well. KEYWORDS artificial neural network, microwave filter, optimization algorithm can be regarded as the forward process from physical

In this letter, we propose an end-to-end inverse modeling and optimization

method for microwave filter designs based on the data-augmentation learning

strategy. Because of the non-uniqueness of solutions, it is difficult to achieve

good convergence with artificial neural networks for inverse designs when the

parameter space is very large. We prove that the accuracy of inverse predic-

tions can be significantly improved using the network's self-generated data

and the optimization can be greatly accelerated with the help of the inverse

network. The predicted structural parameters can be used as initial values for

optimization, which reduces the number of iterations and avoids falling into

structures to EM responses.^{3–7} In this process, sufficient iterations are necessary to ensure convergence and it is limited by the initial values and optimization time. The forward surrogate model has been used to generate data in the design of shunt switches,⁸ where generated data can only be used for the design of one structural parameter at the resonant frequency. Different from the forward process, the inverse design can directly obtain the structural parameters from the design specifications without iterations or prior knowledge.9-12 However, one type of EM response may correspond to many groups of filter structural parameters,¹³ which makes it difficult for the algorithm to converge. Therefore, it easily falls into poor local optima, especially when the parameter space is very large. The multivalued neural network has been proposed to handle this non-uniqueness problem,¹⁴ as they

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can get multiple prediction values from one inverse model. However, large data sets lead to increased runtimes. Regularized deep belief network has been used to extract microwave filter coupling matrices from given *S*-parameters.¹⁰ In this case, the coupling coefficients need to be converted to structure parameters for manufacture, which undermines this method's efficiency.

In this letter, we propose a data-augmentation learning strategy for filter designs that can effectively improve the accuracy of inverse designs when the structural parameter space is large. We use deep learning in an endto-end manner to establish links between physical structures and EM responses. The well-trained forward network is not only a surrogate model but also a data generator that produces more data for the inverse network to learn. This architecture, which uses the data generated from the forward network to train the inverse network, can be called a data-augmentation learning strategy since it can improve the accuracy of inverse predictions. The performance of the inverse network suffers from non-uniqueness problems.¹⁴ Thus, it is difficult to build a completely accurate inverse model. An optimization is added when inverse predictions cannot perfectly meet the requirements. Different from previous works,^{3,4} the inverse model's predictions are used as initial values that can reduce the likelihood of falling into local optima.⁹ We also simplify the objective function so that the target focuses on a few key points, which further improves the optimization speed.

2 | PROPOSED MODELS AND ALGORITHM

An ANN is built for forward predictions. The structural parameters x_1 , x_2 , ..., x_n and frequency x_f are input to the network. To uniformize the parameters' scales, data normalization is first performed as

$$x_m^{\text{input}} = \frac{x_m - x_m^{\min}}{x_m^{\max} - x_m^{\min}} (m = 1, 2, ..., n, f)$$
(1)

where all the input data are scaled to a range between 0 and 1. The output layer is the magnitude of S_{11} which is represented as y^{l}

$$y^{l} = \varphi\left(\sum_{n=1}^{N} \omega_{n}^{l} y_{n}^{l-1} + b^{l}\right)$$

$$\tag{2}$$

where *N* is the total number of neurons in layer l - 1. ω and *b* are the weights and bias, respectively. $\varphi(x)$ is the

LeakyReLU activation function defined as bellow and α is set to 0.3.

$$\varphi(x) = \begin{cases} x, & \text{if } x > 0\\ \alpha x, & \text{if } x \le 0 \end{cases}$$
(3)

The relationship between the physical structure and EM responses is complicated and it can be represented effectively by deep neural networks.^{15,16} The trained forward network can accurately predict the EM responses, which ensures the accuracy of generated data.

Because different combinations of structural parameters may produce similar EM responses, training the inverse network usually does not result in effective convergence. Here, we propose the data-augmentation learning strategy, as shown in Figure 1A. The normalized data are used for the forward network training. After proper weight initialization and the adjustment of other hyperparameters, the well-trained forward network can provide quite accurate EM predictions when compared to simulations. In order to get more data sets, a randomly generated set of structural parameters is firstly input to the trained forward model. The corresponding EM response is then predicted from the structural parameters. This process will be repeated until all the generated data is obtained. Finally, the random structural parameters and predicted EM responses are merged into generated datasets, which can be used together with the simulated datasets for inverse network training. Most importantly, the time needed to generate the data is negligible when compared with simulations, which can be considered a data augmentation method.

The existence of non-unique solutions is the essential feature of inverse problems, and it will not change in the process of simulation or neural networks. Data sets augmentation does not fundamentally solve the non-unique solution problem, but it provides enough data for the neural network to learn and improves the accuracy of inverse predictions. A neural network with strong generalization ability should learn as much as possible the features of the given data and infer equally well on the new data. But there is a premise: the data sets should reflect the probability distribution of the problem's solutions. Therefore, data augmentation is a good way to enrich the features in data sets while maintaining the time required to collect them. Model performance of neural networks improves with the amount of training data.¹⁷ The forward model provides more training data for the inverse which results in its effective network training, convergence.

For the fabrication of filters, structural parameters and the corresponding EM responses are the most proposed algorithm



important concerns. Transfer functions and coupling matrices are intermediate products of the design process, thus additional conversion and data processing for the coupling matrices are needed to complete the filter design.¹⁸ The proposed algorithm is shown in Figure 1B, which is carried out in an end-to-end manner mapping the desired S-parameters to the corresponding physical structures directly. Since transfer functions and coupling matrices are not considered, the proposed end-to-end algorithm can also be employed in other device designs like antennas. The desired S_{11} curve is generated by Chebyshev polynomial. After data-augmentation training, the inverse model generates structure parameters from the required S_{11} target. Then the forward model outputs the predicted S_{11} values corresponding to the inverse predictions. If the predicted S_{11} values meet the design requirements, the structure parameters of the inverse design are output directly. Otherwise, the results of the inverse design will be used as the initial values for the genetic algorithm (GA), and the iterative optimization will be carried out together with the forward model until the requirements are met.

For cavity filters, both the height of the cavity and the length of the resonance rod affect the resonant frequency. Furthermore, different combinations of structural parameters may correspond to very similar EM responses, which will inevitably lead to unpredictable local optima, especially when the solution space is very large. The optimization algorithm depends on the initial values and it will find the optimal solution near them. Choosing good initial values will speed up the convergence and avoid falling into a poor local optimal solution. Compared with using theoretical calculations to obtain the initial values of the filter structure,¹⁸ the neural network only pays attention to the data itself, which can be easily extended to the design of other devices. The data-augmentation learning strategy can make fairly accurate predictions for structural parameters and those can be used as initial values for optimization, which significantly reduces the

size of solution space and the number of required iterations.

A good trade-off between the forward design and inverse design has been completed in our proposed algorithm. The inverse design is less stable because of nonuniqueness problems, but it is very fast. The forward process is limited by the initial structure and multiple iterations are required, but it is stable. It is better to get the design results stably and quickly while maintaining the time cost for collecting data sets.

| PERFORMANCE OF THE 3 ALGORITHM

The fourth-order interdigital cavity filter is used as an example; its geometry is shown in Figure 2A. The design variables are $X = [L_1, L_2, d_{12}, d_{23}]$ where $[L_1, L_2]$ are the lengths of the resonant units and $[d_{12}, d_{23}]$ are the distances between two adjacent units. The frequency range is set to 0.5-4.5 GHz. Nine hundred data samples are simulated and each one contains the structure parameters and S_{11} values. Eight hundred simulated samples are used for building models' training sets, while 100 are used for building testing sets. For one data set of the forward model, the inputs are the normalized structural parameters and one normalized frequency value while the output is the unnormalized S_{11} value at this frequency. The range of designed parameters space is illustrated in Table 1. The relative range is defined as 2 $(X_{\text{Max}} - X_{\text{Min}})/(X_{\text{Max}} + X_{\text{Min}})$ which indicates the size of the parameter space.

The feature extraction capability of a neural network increases with the number of layers, but too many hidden layers can lead to overfitting. After parameters adjustment, the chosen fully connected network (FCN) has 24 hidden layers. The number of input layer neurons, hidden layer neurons, and output layer neurons are 5, 80, and 1 respectively. The information of other parameters



 TABLE 1
 Space range of structure parameters in millimeters

Structure parameters	L_1	L_2	<i>d</i> ₁₂	<i>d</i> ₂₃
Max	48	48.5	3.2	4.7
Min	18	15.5	2	3.2
Relative range	90%	103%	46%	38%

in the network is listed in Table 3. After training the forward network, the simulation results and predictions are almost the same as shown in Figure 2B. The mean absolute error of the S_{11} -parameters at each frequency point is 0.48 dB while experimenting on 100 random structure combinations that are not included in the data sets.

Inverse problems are usually more difficult to solve than forward ones because of non-uniqueness. The inverse model is the modeling of the inverse problem, and the complexity of the problem itself leads to the difficulty of modeling. Therefore, the inverse model requires more trainable parameters than the forward surrogate model, which indicates more data sets are indispensable.

The well-trained forward network can be used as a data generator to produce 3600 samples. The time needed to generate one result is 0.23 s, which is much faster than EM simulation as shown in Table 2. Then, the generated data and simulated data are input into the inverse network for training. The inverse model's architecture is also an FCN with 12 hidden layers. The number of neurons in each hidden layer is 140. For one data set of the inverse model, the inputs are S_{11} values at 251 frequency points, and the output is structure parameters which are also scaled to a range between 0 and 1. The loss function is set to mean squared error. To avoid overfitting, the value of dropout in each hidden layer is set to 0.07. As shown in Table 3, the testing loss is much smaller than that of the network trained on simulated data only, which indicates the accuracy of inverse predictions have been improved

greatly. In Figure 3A, the inverse predictions based on the mixed data sets are more accurate than those based on the simulated data sets. Especially for example 1, the new prediction, which is obtained in less than 1 s, exactly matches the target without any optimizations. Although the inverse prediction in example 2 does not fully meet the target, it is much better than the prediction based on simulation data.

With the help of data augmentation, the accuracy of inverse predictions has been significantly improved. Although the inverse predictions cannot be completely accurate in all situations, more accurate inverse predictions will speed up the optimization. As the example 2 in Figure 3A, the inverse predictions based on the models trained on simulated data sets and mixed data sets are $[L_1, L_2, d_{12}, d_{23}] = [17.598, 15.672, 2.650, 3.757]$ mm and $[L_1, L_2, d_{12}, d_{23}] = [21.095, 18.913, 2.515, 3.804]$ mm. By taking these two sets of structural parameters as initial values, the final optimization results can be obtained as $[L_1, L_2, d_{12}, d_{23}] = [17.121, 16.224, 1.944, 3.509]$ mm and $[L_1, L_2, d_{12}, d_{23}] = [20.810, 18.792, 2.271, 3.434] \text{ mm}$ respectively. As shown in Figure 3B, the optimization result based on the mixed data sets has realized the target. The size of the population in the GA and the number of iterations in optimization 1 and optimization 2 are 20, 15, and 60, 60 respectively. If initial values are not accurate enough, it is difficult to converge in a short time since the optimization algorithm iterates around the initial values.

There is another example to illustrate the details of the optimization. For the design of the fourth-order interdigital cavity filter, the specification of the design goal is | $S_{11}| < -24$ dB in 2.15–3.15 GHz. The predicted structure parameters are $[L_1, L_2, d_{12}, d_{23}] = [23.91, 21.917, 2.405, 3.582]$ mm and the corresponding S_{11} curve is shown in Figure 4A. Although the return loss of the inverse prediction curve meets expectations, the bandwidth is not wide enough. Finding the optimal structural parameters in a

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TABLE 2 Comparison of samples' simulation and generation		Number of samples	Time for one sample	Time for total samples
sinulation and generation	Simulation	900	8.5 s	2.2 h
	Generation	3600	0.23 s	13.8 min

TABLE 3 Parameters comparison of different models

	Data sets	No. of hidden layers	No. of neurons in each hidden layer	Dropout	Loss function	Training loss	Testing loss
Forward model	900 (simulated)	24	80	0.3	Mean square error	0.68	0.80
Inverse model A ^a	900 (simulated)	9	140	0		0.0089	0.0103
Inverse model B ^a	900 (simulated) + 3600 (generated)	12	140	0.07		7.18e-4	8.19e-4

^aInverse model A is trained on simulated data sets and inverse model B is trained on mixed data sets.

FIGURE 3 (A) Inverse predictions based on mixed data (red curves) and simulated data (green curves). Three curves on the left are example 1 and the right ones are example 2. (B) The comparison of the target and optimization results. Optimization 1 is based on the inverse model trained on mixed data sets and Optimization 2 is based on the inverse model trained on simulated data sets





wide range requires considerable time and the result easily falls into poor local optima. The inverse predictions can be used as initial values for optimization, which greatly reduces the size of solution space. The new parameter space is centered on the inverse predictions, and the upper and lower bounds of L_1 , L_2 , d_{12} , and d_{23} are [±0.6, ±0.6, ±0.3, ±0.3] mm respectively. The corresponding relative ranges are 5%, 5.5%, 25%, and 17% for L_1 , L_2 , d_{12} , and d_{23} which are significantly smaller than the values in Table 1.



FIGURE 5 (A) Illustration of more results. The two curves on the left are example 1 and the right ones are example 2. (B) Comparisons of the target, optimization result and measurement

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TABLE 4 Comparisons of ANN-assisted filter designs between recent works and the proposed method

	Methods	Initial values	No. of Iterations	Completion time
Zhao and Wu ³	ANN and homotopy optimization	Filter designer	11	8.3 min
Zhang et al. ⁴	ANN and multiphysics optimization	Filter designer	7	5.8 min
This work	Inverse design	—	—	0.4 s ^a
	ANN and GA optimization	Random	100	4 min ^b
	ANN and GA optimization	Inverse predictions	15	35 s

Abbreviation: ANN, artificial neural network.

^aThe specifications are accomplished under the inverse design.

^bDesign specifications are not accomplished in this time.

Some key points are selected to simplify the objective function in the optimization. As shown in Figure 4B, seven key points are marked on the target curve and the objective function is constructed as

$$F = \begin{cases} \frac{1}{7} \left(\sum_{n=1}^{4} \left| S_n^{\text{tar}} - S_n^{\text{pre}} \right| + \sum_{m=1}^{3} \left| S_m^{\text{tar}} - S_m^{\text{pre}} \right| \right), & \text{if } S_m^{\text{pre}} > S_m^{\text{tar}}(m = 1, 2, 3) \\ \frac{1}{7} \left(\sum_{n=1}^{4} \left| S_n^{\text{tar}} - S_n^{\text{pre}} \right| \right), & \text{if } S_m^{\text{pre}} \le S_m^{\text{tar}}(m = 1, 2, 3) \end{cases}$$

$$(4)$$

where S_n and S_m are the minima and maxima of S_{11} values within the passband. S^{tar} and S^{pre} are the values on the target curve and the predicted one. The objective function is expressed as the mean absolute error for upper points if prediction values from the forward model are higher than the target. Otherwise, it will be set to 0. In this way, the optimization speed can be improved to 30 times when compared with the optimization containing all 251 frequency points. Finally, the specification is realized in 35 s, as shown in Figure 4B. The curves of optimization 1 and optimization 2 are based on the same forward model. The difference is that optimization 1 uses the inverse prediction as initial values, and the initial values of optimization 2 are randomly selected in the space of structure parameters. The optimization result with inverse

predictions as initial values fits well with the lower points and the values of the curve are all smaller than the target in the passband. The optimized structural parameters are $[L_1, L_2, d_{12}, d_{23}] = [24.23, 22.18, 2.232, 3.349]$ mm which are very close to inverse predictions and the deviations are 1.3%, 1.2%, -7.2%, and -6.5%. It is also worth noting that optimization 1 and optimization 2 use the same size of population (20) in the GA, but the number of iterations used for optimization 1 and optimization 2 is 15 and 100 respectively. It means that the optimization can be quickly converged with the help of the inverse network.

The algorithm we proposed is robust and applicable to other relatively high- or low-frequency bandpass filter designs. As shown in Figure 5A, both design results meet the requirements for the bandwidth and return loss. The fabricated filter prototype is measured using a vector network analyzer, shown in Figure 5B, which indicates the proposed method is valid.

As shown in Table 4, ANN and homotopy optimization have been used for waveguide bandpass filter designs and the forward model is just corresponding to sub-structures,³ which is only suitable for filters cascaded by single cavities. Multiphysics optimization technique incorporating ANNs and trust-region algorithm has been developed and the forward model requires additional non-geometric parameters as input such as electric potential.⁴ The input of our proposed method is only structural parameters that can be easily extended to other designs of microwave devices. The completion time in the table refers to the optimization time after the model is trained. Through the comparison with the case using random initial values, the optimization can be quickly converged with the help of the inverse network.

4 | CONCLUSION

We have presented an end-to-end inverse modeling and optimization method for microwave filter designs based on the ANN. The data-augmentation learning strategy has been proposed to improve the precision of filter inverse designs when the parameters space is large. The great amount of data generated from the forward model saves time for collecting data sets, and the inverse predictions become more accurate because of the sufficient data. The predicted structure parameters of the inverse network provide the initial values, which greatly accelerates the optimization. The applications on fourth-order interdigital cavity filter designs show the proposed method is valid over a wide frequency range. It is worth noting that the number of data sets used for training the forward model is slightly larger and better network architecture with fewer data sets is worth exploring.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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