SURROGATE-BASED CONFIGURATION GLOBAL OPTIMIZATION

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ABSTRACT

This study employs machine learning to optimize the electromagnetic field between two microwave sources in a heating cavity, as heating speed is dependent on electromagnetic field strength. We use Ansys HFSS to analyze parameters such as the placement of magnetrons, their phase, the use of WR340 waveguides, the waveguide's direction, and the microwave source frequency. These adjustable parameters, referred to as "points," are optimized using a multi-model Surrogate model to maximize electromagnetic field intensity. The model iteratively exchanges data with Ansys, generating and testing candidate solutions. Suboptimal outcomes are integrated back into the dataset for model refinement. To balance exploration and exploitation, the model uses three sampling methods over five iterations—three local, one medium, and one global. After 1,036 numerical analyses, the optimal electromagnetic field solution found was 159,645 V/m.

Keywords: *global optimization, surrogate model, Ansys HFSS.*

1. INTRODUCTION

With the rise of computer modeling and advanced simulation in industry, Expensive Black-Box Optimization Problems (EBOP) have become prevalent. These problems are often multimodal and computationally intensive, making traditional methods like genetic algorithms costly due to extensive evaluations. Surrogate-based Optimization (SBO) addresses these challenges by using surrogate models to predict and reduce the need for expensive computations, efficiently focusing on promising regions for global optimum solutions.

SBO generally involves three steps: a) selecting initial sample points using Design of Experiments (DoE); b) building surrogate models; and c) updating the models with new promising points. DoE methods include Random, Factorial, and Latin Hypercube sampling. Various surrogate models like Kriging, Radial Basis Function (RBF), and Kernel Partial Least Squares (KPLS) offer unique capabilities for optimization. Combining multiple surrogate models, known as Multiple Surrogate-Based Global Optimization (MSGO), enhances efficiency, accuracy, and robustness.

Balancing global exploration and local exploitation is key in SBO. Effective Infill Criteria help find this balance, ensuring efficient optimization by targeting promising regions while avoiding unnecessary computations.

In industrial applications like designing microwave heating cavities, precise microwave source configuration is challenging and costly with traditional methods. We propose the Surrogate-based Configuration Global Optimization (SCGO) method, using Ansys HFSS for simulation and MSGO to find optimal configurations. Our multi-infill criteria approach improves efficiency by alternately using various sampling methods to identify potential optimal areas. The main contributions of this study are:

- Implementing MSGO combining Kriging and KPLS models. This method fully utilizes the unique advantages of both surrogate models to improve the accuracy and efficiency of optimization.
- Designing Infill Criteria that include three different sampling methods, allowing us to more effectively identify and explore potential areas for global optimum solutions while balancing global exploration and local exploitation.
- Experimentally demonstrating the effectiveness of our method in solving optimization problems of multiple microwave sources in microwave heating cavities, showing the feasibility and effectiveness of our method in practical applications.

The rest of this paper is structured as follows: Section II introduces related works on global optimization. Section III details the proposed SCGO method. Section IV conducts tests related to SCGO. Finally, Section V presents conclusions and future work perspectives.

2. RELATED WORK

2.1. Surrogate-Based Optimization

Surrogate-Based Optimization (SBO) methods have been extensively applied in solving high computational cost optimization problems. SBO reduces the number of expensive objective function evaluations by creating a lower-cost surrogate model that approximates the true objective function [6]. Among these, Radial Basis Function (RBF) is a popular surrogate model, known for its ability to handle nonlinear problems [4]. The Kriging (KRG) model is another commonly used surrogate, appreciated for its interpolation characteristics and high predictive accuracy, especially in cases of sparse data [5]. Additionally, the Kernel Partial Least Squares (KPLS) model combines the advantages of kernel methods and partial least squares, making it particularly suitable for high-dimensional data analysis [10].

2.2. Combining Multiple Surrogate Models

The approach of combining multiple surrogate models has gained widespread attention in recent years. This method aims to amalgamate the strengths of several models to enhance the efficiency and accuracy in solving complex optimization problems [12]. For instance, some studies have combined Kriging and Radial Basis Function (RBF) models, utilizing the high accuracy of Kriging in data interpolation and the capability of RBF in handling nonlinear issues [3]. On the other hand, the combination of Kriging models and Partial Least Squares (PLS) has also shown effectiveness in high-dimensional data analysis, benefiting from the dimension reduction and data compression capabilities of PLS [9].

Additionally, research indicates that combining multiple surrogate models not only improves prediction accuracy but also enhances the generalization capability of the model. This is particularly important for optimization problems with complex objective functions and multiple variables [8]. Therefore, the strategy of combining multiple surrogate models holds significant importance in practical applications, especially in industrial and engineering fields.

2.3. Infill criteria

To boost the predictive precision of surrogate models, incorporating new samples is essential. This approach, known as infill criteria or the adaptive sampling design technique, plays a crucial role in determining the next set of promising samples. The infill criteria aims to navigate the choice of new samples by drawing on the data gathered from the optimization process. It encompasses three strategies: exploitation, which targets areas near the global optimum to refine promising regions; exploration, which searches less sampled or uncertain areas, broadening the search scope; and a hybrid approach that combines both.

In recent years, a diverse range of infill criteria has been devised for the selection of new sample points. The expected improvement [6] is the most well-known single-point criteria, which selects the next sampling point by balancing the exploration of unknown areas with the exploitation of promising regions based on Gaussian Process model predictions. Nonetheless, with the increasing complexity of global optimization problems, the EI method falls short in effectively addressing them. Consequently, [1], [2], [7], [11] design more complicate infill criteria to overcome those problems. For example, [11] applies multi-point infill sampling to update Kriging model. [2] adjusts the search space adaptively.

3. METHOD AND FRAMEWORK

3.1. Initial sampling

SCGO begins by creating an initial set of samples using Design of Experiments (DoE) method. This collected sample data is then used to construct the first surrogate model. Design of Experiments (DoE) incorporates a variety of sampling techniques for effective exploration of the search space. Traditional DoE methods include Random sampling, which involves selecting samples randomly from the population to ensure equal selection probability for each sample; Factorial sampling, which examines all possible combinations of factors and levels in a systematic manner; and Latin Hypercube sampling, a strategy that divides each variable's range into intervals of equal probability and selects samples from these intervals to ensure a more uniform distribution across the range. In this framework, Latin Hypercube sampling is specifically chosen for initial point sampling to align with the goal of gaining insights from each section of the observation plane, thereby fitting our objectives perfectly. Following the generation of initial points, the data is simulated using Ansys HFSS. The outcome of this simulation is the measurement of electric intensity on the observation plane. Subsequently, the measured electric intensity at each point on the observation plane is subjected to averaging. The average electric intensity will be treated as label for the surrogate model.

3.2. Build surrogate model

Following the selection of an appropriate Design of Experiments (DoE) method and conducting simulations with Ansys HFSS, the next phase involves developing a surrogate model to replace the computationally demanding simulations. The surrogate model predicts the average electric field intensity, using 30 candidate points obtained through infill criteria. These predictions are then used to identify the most optimal point for further simulation in Ansys.

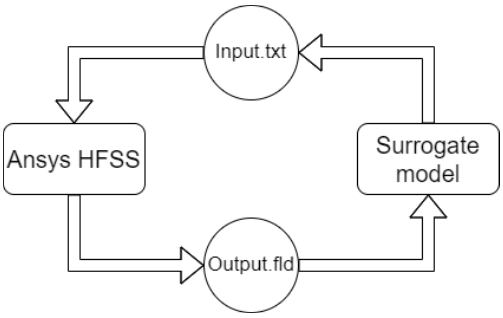

Fig.1 Framework

In this project, we implement Multiple Surrogate-Based Global Optimization (MSGO) methods, using the Kriging and Kernel Partial Least Squares (KPLS) models as surrogates. The Kriging model excels at interpolating unknown data by modeling spatial correlations, making it ideal for accurate predictions of unseen data. The KPLS model, which combines Kernel methods with Partial Least Squares (PLS), is effective for high-dimensional data, handling complex, non-linear relationships by reducing data dimensionality while retaining essential information. Both models are trained on data from the initial sampling stage.

The multimodal approach leverages the unique strengths of each surrogate model, providing multiple perspectives to better understand data distribution. This enhances the analysis by capturing diverse aspects of the data, potentially revealing insights that a single model might miss.

3.2. Infill criteria

The limited quantity of initial points fails to sufficiently capture the breadth of the search space. Additionally, during the initial training phase of the surrogate models using data from the sampling stage, the models may not achieve optimal performance due to the inadequacy of training data. To increase understanding of the search space and enhance the predictive accuracy of these surrogate models, it's necessary to infill new sample points. The process of determining where to place these new sample points is known as infill criteria or adaptive sampling design method. This approach strategically selects additional sample locations to improve the model's understanding of the search space, thereby refining the model's accuracy and effectiveness in the global optimization process.

In this project, we have proposed three distinct infill criteria to enhance the training of our surrogate models. These criteria are categorized as local sampling, medium sampling, and global sampling. Each of these sampling strategies is designed to target different aspects and scales within the search space, thereby providing a comprehensive approach to improve the accuracy and effectiveness of the surrogate models in global optimization tasks.

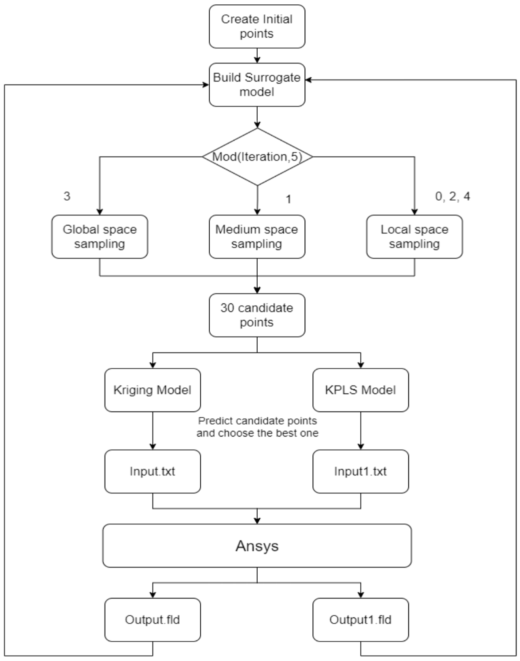

Fig.2 Model Architecture

- Global Sampling: In this strategy, we plan to randomly select thirty points across the entire search space. The primary objective of global sampling is to explore uncharted sections of the search space and to prevent premature convergence to local optima—a frequent challenge in optimization problems. By casting a wide net across the entire search area, the algorithm is less likely to become trapped in a suboptimal solution. This broad exploration aids in ensuring that potential global optima are not overlooked in the optimization process.
- Medium Sampling: This strategy is separated into two parts to accommodate both continuous and discrete parameters in our dataset. For continuous parameters, we initiate the process by identifying the top ten electric intensity values from the dataset. Subsequently, we determine the upper and lower bounds for each continuous parameter. Sampling then occurs randomly within these defined bounds. In contrast, for discrete parameters, our approach involves randomly selecting a category. To illustrate, consider a simple dataset where each data point is represented as [frequency, phase, watts], with frequency being a discrete parameter (options being 3Hz, 2.45Hz, and 2Hz), and the others being continuous. For instance, if we have data points such as [3Hz, 180, 700], [3Hz, 63, 900], and [2.45Hz, 359, 875], the application of medium sampling would proceed as follows:
  1) For the first parameter (frequency), we randomly select from the available discrete options: 3Hz, 2.45Hz, or 2Hz.
  2) For the second parameter (phase), given that the upper bound is 359 and the lower bound is 63, we sample randomly within this range, say between 63 and 359.

3) Similarly, for the third parameter (watts), following the upper and lower bounds from the data (700 to 900), we randomly sample within this range.

Through this method, medium sampling effectively covers a mid-range scope of the search space, balancing exploration and exploitation by focusing on areas around the identified high-performing parameters.

- Local Sampling: This approach begins with the selection of the top ten electric intensity values from the dataset. Following this, we make slight modifications to each of these data points three times. For example, for a degree parameter, we randomly increase or decrease its value by 10 degrees. As a result of these modifications, we generate a total of thirty new data points. The primary objective of the local sampling strategy is to exploit local optima in the search space. By making minor alterations to already high-performing data points, we aim to refine and potentially enhance these points, exploring the immediate vicinity for potentially better results.

During the model's training phase, we dynamically adjust the sampling strategy in accordance with the iteration count. We segment the iterations into units of five: for iterations labeled 0, 2, and 4, we employ local sampling; iteration 1 utilizes a medium strategy, and iteration 3 is designated for global sampling. Employing all three methods in a rotational sequence could potentially uncover superior solutions, as it offers a balanced approach to exploration and exploitation. However, this method is time-intensive. Consequently, to strike a balance between efficiency and performance, we prioritize local sampling, as it has potentially yielded superior results in comparison to other methods. This emphasis on local sampling is justified by its potential to enhance result efficiency, even though there exists a risk of getting trapped in local optima. This approach and its efficacy are substantiated by our experimental findings.

3.3. Refine Model

The infill criteria are designed to generate candidate solutions, and these candidate solutions will be evaluated by surrogate model. The models will predict the electric intensity for each candidate solution. Following this prediction phase, we select the solution with the highest predicted electric intensity from each model. Consequently, in a single iteration, we may end up simulating either one or two solutions, depending on the outcomes predicted by the surrogate models.

These selected solutions are then processed through Ansys HFSS to obtain their actual electric intensities. If the results from Ansys HFSS do not meet our predefined termination criteria. This updated dataset is used to retrain the surrogate models, thereby enhancing their predictive capabilities for future iterations. This iterative process of generating, evaluating, and refining solutions ensures a continuous improvement in the search for optimal solutions within the specified criteria.

3.4. Framework introduction

Our framework comprises two principal components. The first is the surrogate model, which is responsible for generating the parameters that will be utilized in simulations conducted by the second component, Ansys HFSS. Ansys HFSS is a sophisticated 3D high-frequency structure simulation software, designed to simulate electric fields and their interactions with physical structures.

In the simulation process, Ansys HFSS generates output that includes the electric intensity at each point on the observation plane. This output is then processed to determine the average electric intensity, which serves as the target metric for each data set in our study.

If the results from the Ansys HFSS simulations not meet our established termination criteria the new data obtained from these results will be integrated into our existing dataset. This integration is a crucial step, as it allows for the continuous refinement and improvement of the surrogate model. The enhanced model will then be better equipped in future iterations to produce more accurate parameter predictions for subsequent Ansys HFSS simulations, thus creating a cyclic process of optimization and refinement until the termination criteria are satisfactorily met.

4. EXPERIMENTS

4.1. Experimental Setup

In this section, we will describe the implementation detail of the experiment, explain the interaction process between the surrogate model and Ansys HFSS, and outline all the variable parameters required for the simulation.

4.1.1. Interaction Process

After the surrogate model generates the parameters, we apply these parameters by adjusting the Python automation script of Ansys HFSS to automatically complete all operations in Ansys HFSS. Specifically, our automation process includes:

1) Creating a new project;
2) Generating the 3D model of the microwave device;

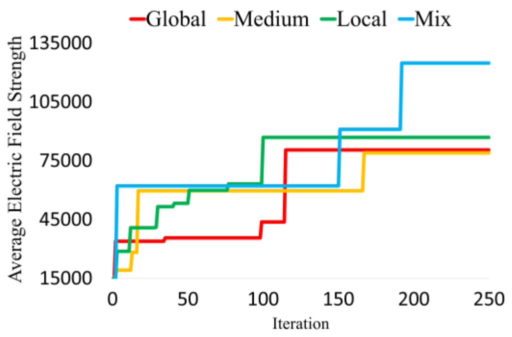

Fig.3 Sampling technique evaluation

3) Setting the simulation physical parameters (material of the device, microwave frequency, etc.);
4) Performing electromagnetic field simulation;
5) Exporting the simulation results.

The final step of exporting simulation results from Ansys HFSS is in the form of a .fld file. Once the surrogate model receives the new simulation results, it integrates these results into the dataset, preparing for the next round of calculations.

4.1.2. Variable Parameters

We first describe the specification parameters of the 3D model. The 3D model of the microwave device is a hollow cube, with the dimensions of the cavity (length, width, height) being variable parameters. We install two magnetrons, fixed on the top and the back side of the device, to provide microwave sources. The wave port position of the magnetrons can be adjusted as well. This parameter represents the offset of the magnetron from the center of the plane. The direction of the wave port from the magnetron is a categorical parameters, which can be adjusted to either horizontal or vertical.

Next, we will describe the physical parameters related to the simulation. The wave port frequency and phase of the magnetron are adjustable. The wave port frequency is a categorical parameters with three options: 2GHz, 2.45GHz and 3GHz, while the wave port phase can be continuously adjusted between 0 degrees and 360 degrees. The material of the microwave device is set to copper.

4.1.3. Simulation Results

We set up a horizontal observation plane at the center of the microwave device, which does not possess physical properties; its purpose is to capture the electric field intensity inside the device. The obtained electric field intensity data will be exported to a .fld file. In this file, the electric field values on the observation plane are organized in a grid pattern, with each points representing the electric field intensity at a specific location on the observation plane. The spacing between these cells is uniformly set to 1 millimeter. We calculate the average of the electric field values for all points on this grid as an evaluation metric for the study.

4.2. Results

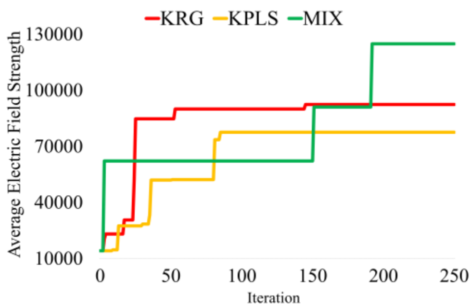

Fig.4 Model performance evaluation

4.2.1. Optimization Impact Assessment

To demonstrate the efficacy of our proposed method, we conducted a comparative analysis by randomly sampling parameters and contrasting them with optimized parameters. Table 1 shows both the randomly sampled and optimized parameters. Note that we run around 1,000 iterations to get the result. It becomes evident that the application of optimized parameters significantly enhances the outcomes. The average electric field strength increase about 50%.

4.2.2. Evaluation of Sampling Methodologies

In the proposed method, we have developed three distinct sampling techniques to generate candidate solutions. This section aims to demonstrate that combining these sampling methods effectively enhances performance. For this purpose, we conducted a

comparative analysis of a mixed version incorporating all three methods and the individual application of each method over 250 iterations. Fig. 3 clearly illustrates that the integration of the three sampling methods achieves approximately 130,000 V/m, whereas utilizing a single sampling method yields a maximum of around 80,000 V/m. Note that Fig. 3 shows the best solution in training dataset.

Furthermore, it is evident that local sampling outperforms both global and medium sampling. The primary reason for this enhanced performance is that local sampling concentrates on exploitation, which involves an intensive search in the vicinity of the current best solution to determine if more optimal solutions exist. This targeted approach allows for a more thorough exploration of promising areas in the solution space, leading to potentially better outcomes.

4.2.3. Model Performance Evaluation

In our proposed method, we have implemented both Kriging and KPLS models as surrogate models. This section is dedicated to illustrating that the concurrent utilization of both models yields superior solutions compared to employing a single model. To validate this

Table 1. Random and Optimized Parameters

	Random Parameters	Optimized Parameters
Cavity Length	398.70 mm	322.73 mm
Cavity Width	359.41 mm	343.44 mm
Cavity High	463.79 mm	308.14 mm
Wave port 1 direction	Horizontal	Horizontal
Wave port 2 direction	Horizontal	Horizontal
Wave port 1 position (X, Y)	(99.82mm, 44.75mm)	(-0.7784mm, -97.2755mm)
Wave port 2 position (X, Y)	(17.71mm, -12.95mm)	(-4.9095mm, 91.1947mm)
Wave port Frequency	2.0Gz	2.45Gz
Wave port 1 phrase	195.83°	27.0739°
Wave port 2 phrase	72.42°	-12.5769°
Avg. Electric Field Strength	7647.59 V/m	159645 V/m

assertion, we conducted a comparative analysis, contrasting the performance of a multi-model approach with each individual model over a span of 250 iterations. Fig. 4 clearly depicts that the multi-model approach is capable of achieving approximately 13,000 V/m, while the application of a single model falls short of reaching even 10,000 V/m. It is important to note that Fig. 4 represents the best solutions found within the training dataset.

5. CONCLUSION

This study presents a surrogate-based configuration global optimization (SCGO) method that optimizes the electric field strength in a microwave device. By using Multiple Surrogate-Based Global Optimization (MSGO), combining Kriging and Kernel Partial Least Squares (KPLS) models, the method improves accuracy and efficiency. An innovative infill criteria strategy, which includes local, medium, and global sampling methods, balances global exploration and local exploitation. Experimental results show a 50% increase in average electric field strength, proving the method's effectiveness. The SCGO method offers a robust solution for complex optimization problems and is applicable to various engineering fields.

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