

# A Numerical Evaluation of an Infill Sampling Criterion in Artificial Neural Network-Based Optimization

Han Li, Leonardo Gutierrez, Masakazu Kobayashi, Osamu Kuwazuru, Hiroyuki Toda, and Rafael Batres

**Abstract**—Surrogate models can be used to replace expensive computer simulations for the purposes of optimization. In this paper, we propose an optimization approach based on artificial neural network (ANN) surrogate models and infill sampling criteria (ISC) strategy to evaluate design variables. The criterion for infill sample selection is a function which aims at identifying design that offer potential improvement. We employ four widely used analytical benchmark problems to test the proposed approach. Our results show that a more accurate surrogate model obtained with fewer points is obtained when one includes the infill sample criterion to an ANN-based optimization.

**Index Terms**—Surrogate model, design variables, artificial neural network, infill sampling criteria, optimization, benchmark function.

## I. INTRODUCTION

Optimization methods for black-box systems have applications in many engineering-domains. Most engineering design problems require high fidelity simulations to evaluate design variables. These simulations are based on mathematical models of some system of interest. Examples include finite element analysis (FEA) method for structural engineering problems or Navier-Stokes models in computational fluid dynamics (CFD). However, for many real world problems, despite steady advances in computing power, a single simulation can take many minutes, hours, or even days to complete. As a result, design optimization becomes impractical since it may require thousands or even millions of simulation evaluations. For example, in order to find the optimal material parameters, the finite element analysis (FEA) along with nanoindentation test is undertaken [1]-[3].

Therefore, to overcome this problem cheap approximating models (often termed “surrogate models”) are sought. These are based on a limited number of calls to the high fidelity model. Once constructed, the surrogate model can replace the original high fidelity model for the purposes of optimization. Polynomial regression [4]-[6], radial basis function (RBF) [7], and Kriging [8], [9] are among some of the most

prominent and commonly used techniques. In this paper we concentrate on artificial neural network (ANN) surrogate models. ANN models have been successfully applied to many engineering problems. ANNs are universal approximators which have been mathematically proven to be able to approximate any continuous nonlinear function arbitrarily well over a compact interval to any degree of accuracy as long as they contain at least one hidden layer.

During an ANN-based optimization, the global optimum will not be found if we only utilize the ANN models built from a small set of initially sampled data, since the models are not globally accurate. Therefore, several new inputs should be added so that the ANN models can be updated, where each new input incorporates with all prior information. This process is performed by the infill sampling criterion (ISC) function. ISC function can adaptively select better additional sampling point to improve the surrogate model and find the optimum value at every iteration. This step is repeated until a time limit, evaluation budget, convergence, or model accuracy is reached.

Since the iterative strategy represents the heart of the surrogate-based optimization process, the choice of ISC is then of great importance. In [10], the expected improvement (EI) is introduced. Also, Viana [11] used the probability of improvement (PI) to update a Kriging surrogate model.

In this paper, we propose a criterion for infill sample selection that helps to select the points in the design space with the biggest contribution to the current error. In other words, it considers both the spatial position of the design variables and the areas of high estimated approximation error generated by the surrogate model. This criterion is simple and easy to use.

The rest of this paper is organized as follows. Section II introduces the setting of this problem. The proposed methodology is presented in Section III. Section IV we show some results from our approach and in the final section conclusions are drawn and areas of further research highlighted.

## II. PROBLEM SETTING

We consider the system of interest as a black box that provides no information other than the measurements of system performance. In a typical approximation model the relationship between responses and design variables on a  $k$ -dimensional domain  $D$  is expressed as

$$y = f(\mathbf{x}, u), \quad (1)$$

where  $y$  is the observed response,  $\mathbf{x}$  is a vector of  $k$

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independent design variables whose values are unknown, and  $u$  is a vector of design parameters whose values are fixed as a part of the problem specifications. In the case of a high fidelity model (such as FEA), the design parameters are assigned values, that is the response  $y$  must be a function  $f_L$  of the parameters  $x$  and  $u$ :

$$y = f_L(x, u). \quad (2)$$

Assuming that we can afford to run the high fidelity analysis  $N$  times, we sample for  $N$  designs denoted by  $((x^{(1)}, u), (x^{(2)}, u), \dots, (x^{(N)}, u))$ , at which we obtain the responses  $(y^{(1)}, y^{(2)}, \dots, y^{(N)})$ . The surrogate model is built on these designs and responses.

The surrogate-based optimization problem is formulated as:

$$\begin{aligned} \text{Min } E_u |f(x, u) - z(x, u)|, \\ \text{s.t. } x \in D \subseteq X^k \end{aligned} \quad (3)$$

where  $E_u$  denotes the expectation with respect to  $u$ ,  $f(x, u)$  is the experiment response,  $z(x, u)$  is the prediction obtained by ANN model, and  $D$  is the design space.

When the probabilistic distribution function  $\varphi(u)$  is given,  $E_u$  is calculated by the following equation:

$$E_u = \int \varphi(u) |f(x, u) - z(x, u)| du. \quad (4)$$

On the other hand, when the uncertain parameters deviate randomly within a certain interval, or the probabilistic distribution function is not given explicitly, the above computation is substituted by the average over  $m$  samples. In this case, a large number of samples can increase the accuracy of such a computation:

$$E_u = \sum_{i=1}^m |f(x, u_i) - z(x, u_i)|. \quad (5)$$

### III. METHODOLOGY

In this section, the methodological foundations of our approach are introduced. The flowchart for the optimization method based on ANN with ISC is shown in Fig. 1. The first step is to generate an initial data set based on some design of experiments. A surrogate model is then built based on true simulations from this initial sample. The second stage extracts knowledge from the surrogate to find points for model refinement referred to as updating. These update points are selected via an infill sampling criterion.

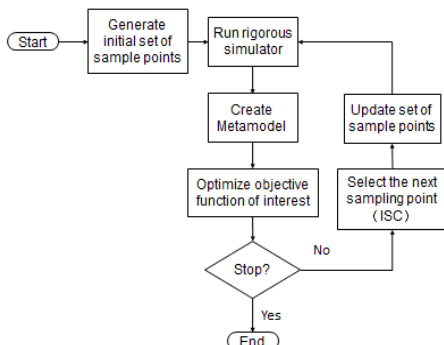


Fig. 1. Flowchart for ANN with ISC.

#### A. Sampling Plan

The first step consists of generating an initial population of design points either by random generation or by means of design of experiments (DOE) techniques [12]. DOE is the preferred sampling plan as it permits to evenly fill the design space with a limited number of points.

The most frequently used techniques in this stage of the process are latin hypercube sampling algorithm (LHS) [13], full-factorial design, orthogonal arrays and box-behnken design. Each of these methods has its own advantages and disadvantages depending on the characteristics of the design problem. Here, we use LHS design optimized with respect to the maximum criterion, which is common choice in many cases. The advantage of this method is that they divide uniformly the design space for each parameter and guarantee to have good space-filling properties.

Then, high fidelity model is executed for all the values of the input variables in the DOE specified in the previous step.

#### B. Building a Surrogate

After selecting the initial sample points an appropriate experimental design and performing the necessary computer runs, the next step is to build surrogate model. Surrogate model is the key to surrogate-based design optimization.

There are several approaches for building such models, here we choose to work with ANNs on the grounds that their training is inexpensive, yet, as we will see, they are sufficiently accurate for optimization purposes.

ANNs are computational models inspired by animal central nervous systems (in particular the brain) that are capable of machine learning and pattern recognition. ANNs can be seen as systems of interconnected "neurons" that can compute values from inputs by feeding information through the network. Three training methods are commonly used, namely back propagation, conjugate gradient, and Levenberg-Marquardt methods.

In Fig. 2, a sketch of a hierarchical neural network is shown. An ANN is a multilayered construction made up of one or more hidden layers placed between the input and output layers. The layers include several processing units called neurons. All of them are connected with variable weights that have to be determined.

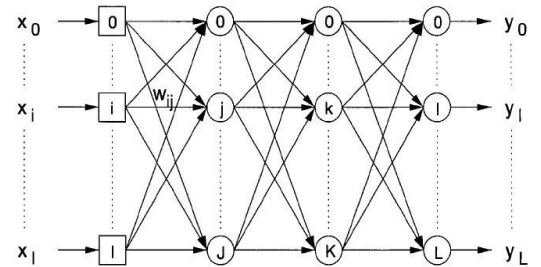


Fig. 2. Sketch of a multilayer feed forward neural net.

The inputs are operated and transformed into the output by the state transition rule as

$$v_j = \sum w_{i,j} y_i + \theta_j, \quad (6)$$

$$y_j = f(v_j), \quad (7)$$

where  $y_i$  in "(3)" and  $y_j$  in "(4)" denote the output from a

neuron  $i$  acting as an input on neuron  $j$  and the output of neuron  $j$  respectively.  $w_{i,j}$  is the synaptic weight,  $\theta_j$  is the bias, and  $v_j$  is the state variable of the synaptic weights which imply the connection strength between the neurons. A neuron in the network produces its output  $y_j$  by processing the net input through an activation (transfer) function  $f$ . In this work, the activation function is given by the smooth sigmoidal function

$$f(v_j) = 1/\{1 + \exp(-v_j)\} \quad (8)$$

taking values between 0 and 1.

An ANN is trained by repeatedly presenting a series of input and output pattern sets to the network. The neural network gradually “learns” the relationship of interest by modifying the weights between its neurons to minimize the error between the actual and predicted output patterns of the training set. Then, a separate set of data called the test set to monitor network’s performance. During training, the learning rule is used to iteratively adjust the weights and biases of the network in order to move the network outputs closer to the target values by minimizing the network performance indicator.

### C. Infill Sampling Criterion

The cornerstone of any optimization strategy based on surrogate models is the choice of the updating method, *i.e.* given an initial global model, how to select the next sites where the expensive objective will be sampled. Perhaps the most obvious strategy is to re-sample in areas that appear promising in terms of the objective function value which predicted by the surrogate model. The success of this approach depends on the quality of the initial approximation. If the initial approximation is accurate, it is likely to lead the designer quickly to the global minimum or at least to a very good solution.

A second approach is to search areas of high estimated approximation error, *i.e.* in our case, to choose the design that maximizes the estimated error of the ANN predictor. This infill criterion uses information of the current model in order to assess the utility of evaluating this design on the actual problem. The infill criteria are used to increase the accuracy of the prediction by creating globally accurate surrogate models.

The offset (error) value  $I_z(p)$  is as a quality index, which is the sum of the difference between the actual response and simulation data. In order to calculate this, we make a sampling, more precisely,

$$I_z(p) = \sqrt{\frac{1}{m} \sum_{i=1}^m (z(u_i, p) - f(u_i, p))^2}, \quad (9)$$

here,  $f(u_i)$  is the actual response at points  $u_i$ , the function  $z$  is a ANN model trained, and  $m$  is the number of experiment data related to the fix parameter  $u$ .

We try to select points with the biggest contribution to the current error. In order to estimate the representativeness of selected point  $p$ , we give a weight function, that is

$$w_{i,j} = d(p_i, p_j) \quad (10)$$

where  $d(p_i, p_j) = 1 - \exp(-\|p_i - p_j\|^2)$ , and  $p_j$  is the original LHS data. This weight function gives the similarity of the design variables. When the two design variables are near each other, the value of this function is small; on the contrary, the two design variables are far away, the value is big.

Based on the above equations, the proposed ISC is given by:

$$p_i = \operatorname{argmax}_{p \in D} \sum_{j=1}^n w_{i,j} (I(p_i) - I(p_j)) . \quad (11)$$

The proposed ISC has the following advantages: 1) it can intelligently add sample points to improve the ANNs, so it can learn with a small number of expensive simulations; 2) it can avoid searching the areas with relative large function values and decrease the computational cost; 3) it considers both the similarity of the design variables and the points of high estimated approximation error which generated by ANN model; 4) It is simple and easy to use.

## IV. EXPERIMENTAL RESULTS AND DISCUSSION

In this section, we employed four widely used analytical benchmark problems [14], namely Rosenbrock, Sphere, Six Hump Camel Back functions of 2-dimensional (2D), and 4D Sphere function.

The benchmark functions are chosen to cover a large variety of problem properties. Rosenbrock (2D) and Sphere (2D) functions are unimodal functions. The valley of the global minimum is easy to find, however fine convergence to the global minimum is difficult. Six Hump Camel Back (2D) is a multimodal function. Also, the simulation is conducted on the 4D Sphere function to account for multiple parameters.

We use LHS to generate the initial sample in all cases. In some cases, by pure luck, this initial sample may include a point close to the global optimum, accelerating the search. To avoid any bias when testing, here ANN and ANN with ISC use the same initial sample. In our setup, the simulation and training of the ANN have been performed using the Neuroet toolbox [15]. Furthermore, the transfer function between the input layer and the hidden layer is “log-sigmoid”, while the transfer function between the hidden layer and the output layer is “pure-linear”. A genetic algorithm is used for both objective-function of interest and for the maximization of ISC.

The performance of the infill criteria can be assessed in a number of ways. Here this performance is measured by the distance of the best finding optimum to the global optimum. To be more precise, for benchmark functions, the true optimum  $x^*$  is known, an intuitive method of comparison is to find the absolute error between the true optimum  $x^*$ , and best feasible point  $x^{best}$ . The absolute error is defined as:

$$\|x^* - x^{best}\| = \sqrt{(x^* - x^{best})^2}. \quad (12)$$

A series of 20 runs was performed for each of the 4 test functions. This was done to see at what low evaluation number each method approached convergence for all 20 runs. With that setup, the global optima of the criteria are found in

the vast majority of the cases for all considered configurations.

#### A. Sphere Function (2D)

The first example is the minimization of the Sphere test function, a common and simple benchmark test function used in surrogate-based global optimization. It is given as  $f(x) = x_1^2 + x_2^2$ . Test area is usually restricted to hypercube  $-5.12 \leq x_i \leq 5.12$ ,  $i = 1, 2$ . It is continuous, convex and unimodal. The Fig. 3 shows its two-dimensional form. There is a global optima of the Sphere function, for which  $f(x^*) = 0, x^* = (0,0)$ .

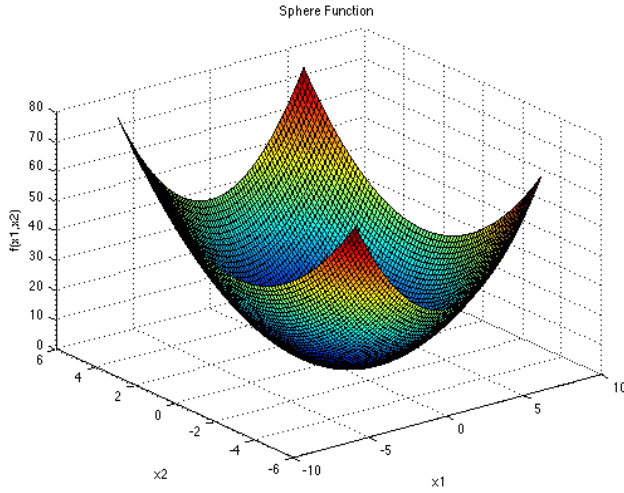


Fig. 3. Sphere function in 2D.

TABLE I: COMPARISON OF ERRORS FOR SPHERE FUNCTION (2D)

Method	The number of sample points $m$	The values of the finding optima	Average error
ANN	10	(-1.127472, 0.324886)	1.376740
ANN	30	(6.36508E-5, -0.008073)	6.51796E-05
ANN	35	(-0.0094507, -0.005342)	1.17858E-04
ANN	40	(-0.0072253, -0.003513)	6.45475E-05
ANN with ISC	11	(-0.465341, -0.217933)	0.264037
ANN with ISC	15	(0.098401, -0.064587)	0.013854
ANN with ISC	16	(-0.015163, 0.009281)	3.16055E-04
ANN with ISC	18	(0.001937, -0.00234)	9.22623E-06

We select an initial design with  $m = 10$  points. Table I shows the results of both ANN and ANN with ISC approaches. It can be seen that as  $m$  increases, our model generally becomes more accurate (the error reduces), as expected. Here we compare the accuracy of the optimum of the true function with and without ISC. Both approaches succeed in finding the true optimum. Without ISC the ANN required around 40 data points to reach the global optimum. On the other hand, utilizing the proposed ISC the optimum was found with only 18 points after 8 iterations. So in this case, ANN with ISC is far superior.

#### B. Six-Hump Camel Back Function (2D)

Six-Hump Camel back function (2D) is defined as:

$$f(x) = 4x_1^2 - 2.1x_1^4 + \frac{x_1^6}{3} + x_1x_2 - 4x_2^2 + 4x_2^4.$$

Test area is usually restricted to  $-5 \leq x_i \leq 5, i = 1, 2$ .

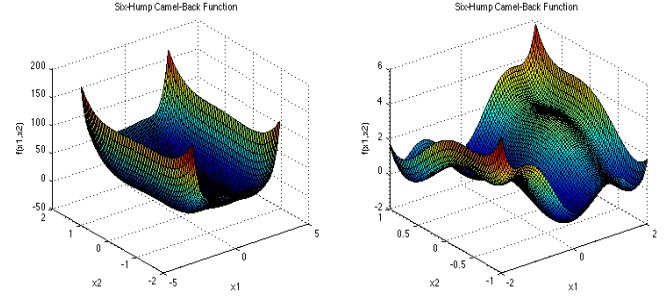


Fig. 4. Six Hump Camel Back Function in different range.

The left plot in Fig. 4 shows the six-hump Camel function on its recommended input domain. The plot on the right shows only a portion of this domain, to allow for easier viewing of the function's key characteristics.

In the continuous domain, six local minima are located, two of them are global minima; namely,  $x^* = (0.089842, -0.712656)$  and  $x^{**} = (-0.089842, 0.712656)$  with  $f(x^*) = f(x^{**}) = -1.031628$ . It also has two additional local minima.

We select an initial design with  $m=30$  points. Table II shows the results of both ANN and ANN with ISC approaches. Since this test function is complicated, the results of both methods are not entirely accurate. In some cases, the optimization method gets trapped in one of the local minima. Still, the use of the ISC took nearly 36 points for an acceptable solution. Without the ISC, a similar solution was found after 45 points.

TABLE II: COMPARISON OF ERRORS FOR SIX-HUMP CAMEL BACK FUNCTION (2D)

Method	The number of sample points $m$	The values of the finding optima	Average error
ANN	30	(1.833207, 0.269188)	1.395452
ANN	35	(0.989603, 1.410874)	0.909037
ANN	40	(0.340639, 0.130975)	0.511647
ANN	45	(-0.813648, 0.218690)	0.619639
ANN with ISC	31	(1.840641, 0.107743)	1.367189
ANN with ISC	35	(0.0954703, 0.004843)	0.507324
ANN with ISC	36	(0.270422, -0.05306)	0.483538
ANN with ISC	38	(0.409892, 0.328426)	0.445692

#### C. Rosenbrock Function (2D)

The Rosenbrock's valley is a classic optimization problem, known as banana function or the second function of De Jong. It is naturally nonseparable and is defined as follows:

$$f(x) = 100 \times (x_2 - x_1^2) + (1 - x_1)^2.$$

Test area is usually restricted to  $-2.048 \leq x_i \leq 2.048, i = 1, 2$ .

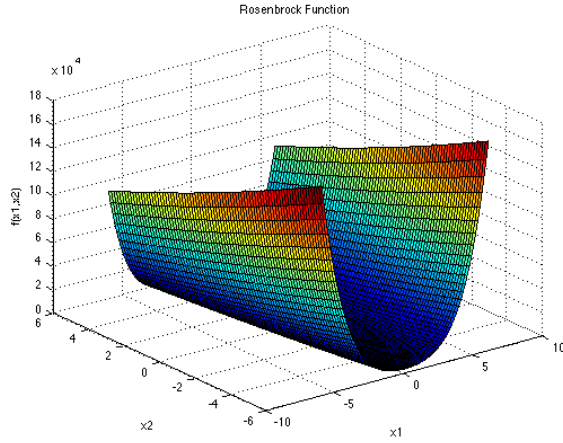


Fig. 5. Rosenbrock function in 2D.

Rosenbrock function (2D) has a global minima  $x^* = (1,1)$  with  $f(x^*) = 0$ . The global minimum is inside a long, narrow, parabolic shaped flat valley. To find the valley is trivial. To converge to the global minimum, however, is difficult.

Similar to the previous cases,  $m=30$  points were selected as initial design and the results are given in Table III. We can see from the table, that the use of the ISC permitted the optimization algorithm to find a solution near to the optimum with a small number of points (36 points). However, we observed very little success at finding optima by ANN with LHS design alone. The optimization algorithm was unable to make any additional progress beyond this point, perhaps struggling to traverse the valley.

TABLE III: COMPARISON OF ERRORS FOR ROSENBRICK FUNCTION (2D)

Method	The number of sample points $m$	The values of the finding optima	Average error
ANN	30	(0.326942, 0.408716)	0.895891
ANN	35	(-0.10094, 0.070638)	1.440765
ANN	40	(0.584282, 0.254416)	0.853649
ANN	45	(0.547114, 0.299495)	0.834154
ANN	50	(0.593662, 0.207915)	0.89023
ANN with ISC	31	(-0.312919, 0.229329)	1.522397
ANN with ISC	35	(0.909437, 0.954252)	0.101461
ANN with ISC	36	(0.804714, 0.947936)	0.202112
ANN with ISC	38	(1.006475, 1.018454)	0.019561

#### D. Sphere Function (4D)

The Sphere function (4D) has four parameters. The function is defined as:  $f(x) = x_1^2 + x_2^2 + x_3^2 + x_4^2$ ,  $-2 \leq x_i \leq 2, i = 1, \dots, 4$ .

TABLE IV: COMPARISON OF ERRORS FOR SPHERE FUNCTION (4D)

Method	The number of sample points $m$	The values of the finding optima	Average error
ANN	20	(1.099, 2, 2, 1.71)	3.483605
ANN	40	(-0.0537, 0.00576, -0.0285, -0.3004)	0.306571
ANN	50	(0.03244, -0.01353, -0.06338, 0.13806)	0.155925
ANN	55	(-0.00164, 0.04242, 0.09037, 0.00972)	0.100317
ANN with ISC	21	(-0.3707, -1.999, -2, 0.3936)	2.879635
ANN with ISC	23	(-0.1786, -0.183, -0.0633, 0.0728)	0.273351
ANN with ISC	26	(-0.0093, -0.1436, -0.1662, -0.1478)	0.264952
ANN with ISC	28	(-0.0085, -0.09655, -0.06465, -0.1295)	0.171102

From Table IV, the results in 4D sphere function are similar to 2D case. Both approaches succeed in finding the true optimum. However, less sample points are required if the ISC guides the selection of the design points to be sampled.

To summarize the results, boxplots for the sphere 4D, six-hump camel, and Rosenbrock function are presented in Fig. 6 and Fig. 7 which are more visualized. Fig. 6 presents the results with ISC and the Fig. 7 without ISC method. It turns out that use of ISC has a superior performance on all benchmark functions.

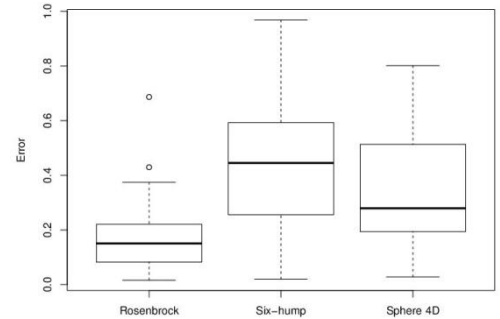


Fig. 6. Boxplot of the errors by ANN with ISC method over 20 runs.

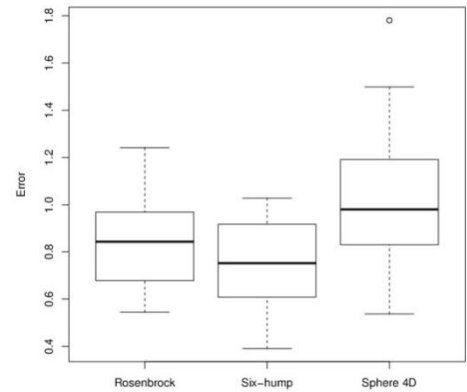


Fig. 7. Boxplot of the errors by ANN method over 20 runs.

#### V. CONCLUSION AND FUTURE WORK

In this paper, an optimization method using ANN with ISC is developed. A predictive model including design



parameters is built by using ANN with ISC to reduce the computational time. By comparing ANN and ANN with ISC methods based on a benchmark with a variety of test functions, we get the results showing that the proposed method can identify and calculate design parameters with a minimum number of computer simulations.

It must be mentioned that the proposed ISC assumes that the design space is fixed, and the range of variables is based only on the criteria of the experienced researchers in their related fields. Further to this, by selecting model update points is close proximity to the constraint boundaries, the regions that are likely to contain the feasible optimum can be better modeled. Thus, a changeable design space will be taken into consideration in research.

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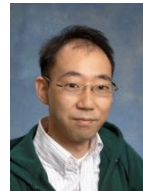
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