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Construction of the radial basis function based on a sequential sampling approach using cross-validation †

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Abstract

Metamodels have been widely used in engineering design to replace the high-fidelity simulations which lead to high computation costs. The accuracy of a metamodel is strongly affected by the sampling strategies. Most strategies use the Kriging as a metamodel since it provides information on the prediction error. In this paper, a new sequential sampling approach is proposed, which is capable of employing many other metamodels: it is not restricted within Kriging. It selects additional points by two ways according to the number of sampling points. The capabilities of the proposed approach have been demonstrated by test problems with various features.

Keywords: Cross-validation; Design of experiments; Radial basis function; Sequential sampling

1. Introduction

Although the computational power has been dramatically improved in over the past decades, iterative design optimizations or reliability-based design optimizations (RBDO) often have computational limitations. This is because considerable computational time is still necessary for complex nonlinear simulation analysis, such as the collision analysis and the flow field analysis. To overcome such practical limitations, various researches on utilizing the metamodels [1] to approximate the complex and computationally expensive simulation models [2-4] are in progress.

The accuracy of a metamodel depends highly on the metamodeling technique and the characteristics of the original function, which is directly related to the sampling approach. Koehler and Owen [5] provided a good review on various computer-based experiments. Typically, the sample points are generated all at once, or in other words, at one-stage. On the contrary, the sequential sampling approach generates sample points one after another according to the particular criteria instead of generating all points at once. In sequential sampling technique, the new sampling points and corresponding responses are sequentially updated. Therefore, the sequential sampling approach has significant advantages. For example, it can use the previously generated information of the metamodel, and the sampling process can be stopped as soon as there is sufficient information [6]. Namely, sequential sampling is the technique developed for both improving the efficiency of a design of experiments (DOE) and the accuracy of metamodels.

The study presented in this paper focuses on investigation into the sequential sampling for global metamodeling in order to improve the accuracy of a metamodel over the entire design space of interest. There are several sequential sampling techniques: maximin distance approach that maximizes the minimum distance between the existing sample points [7], Entropy approach that sequentially adds sample

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points, which maximizes the entropy [8], mean square error (MSE) approach that uses prediction error of Kriging model [6], sensitivity approach that adds sample points sequentially at the peak points of the metamodel [9] and the cross-validation approach that adds sample points at the location where the cross-validation error is maximized [10].

In the metamodel application, the MSE method and the integration mean square error (IMSE) approach are the most widely used methods among the existing sequential sampling methods, which are limited to Kriging. Researches on sequential sampling methods, which are not restricted by metamodeling techniques, are still under study. Among them, a representative one is the cross-validation approach that does not require additional sampling points [10].

This paper proposes a sequential sampling method, which is applicable to any metamodel and is able to improve the accuracy of the resulting metamodel with the existing cross-validation approach. The proposed approach is applied to various mathematical problems and the accuracy of the approach is evaluated by comparing it to other sampling methods.

2. Sequential sampling approaches for global metamodeling

2.1 Metamodeling techniques

2.1.1 Kriging

A Kriging model [6] represents the information obtained from the numerical experiments as a summation of a global model and local deviation, given by Eq. (1):

$$y(\mathbf{x}) = \mathbf{f}(\mathbf{x})\boldsymbol{\beta} + Z(\mathbf{x}) \tag{1}$$

where, $Z(\mathbf{x})$ is a normal distribution with a mean of 0 and a variance of σ^2. The deviation for each sampling point has correlation defined by Eq. (2):

$$Cov\left[Z(\mathbf{x}_i), Z(\mathbf{x}_j)\right] = \sigma^2 \mathbf{R}\left[R(\mathbf{x}_i, \mathbf{x}_j)\right],\ i, j = 1, \cdots, N$$
$$R(\mathbf{x}_i, \mathbf{x}_j) = \exp\left[-\sum_{k=1}^{n_{dv}} \theta_k \left| x_{i,k} - x_{j,k} \right|^2\right] \tag{2}$$

where, N and n_{dv} are the number of sampling points and the number of design variables, respectively. $x_{i,k}$ is the value of the k th design variable at the i th sampling point. $R(\mathbf{x}_i, \mathbf{x}_j)$ is a function that represents the correlation between two sampling points, $\mathbf{x}_i$ and $\mathbf{x}_j$. Typically, $R(\mathbf{x}_i, \mathbf{x}_j)$ is defined as a Gaussian correlation function. In Eq. (2), the unknown correlation coefficient θ_k can be found by the global optimization using the maximum likelihood estimation (MLE) method.

The Kriging technique is very flexible in capturing nonlinear behaviors of the model because the correlation functions can be statistically tuned by the sample data. Another good feature of Kriging is its ability to provide an estimation of the prediction error, which is the essence of several sequential approaches. However, since the calculation of the correlation requires the global optimization, it consumes significant computational power and time for problems with many design variables and sampling points. Another shortcoming of this technique is that it may fail to generate the proper metamodel if the global optimization cannot be successfully accomplished.

2.1.2 Radial Basis Function (RBF)

RBF [11, 12] is often used to perform the interpolation of scattered multivariate data. The metamodel appears as a linear combination of Euclidean distances and weights, given by Eq. (3).

$$\hat{y}(\mathbf{x}) = \sum_{i=1}^{N} w_i \varphi_i(\mathbf{x}, \mathbf{x}_i) \tag{3}$$

where, N is the number of sampling points, w_i is the weight determined by least-squares method and $\varphi_i(\mathbf{x}, \mathbf{x}_i)$ is the i th basis function determined at the sampling point $\mathbf{x}_i$. Various symmetric radial functions used as the basis function are listed in Table 1.

The RBF method is known to be a good interpolation method like the Kriging. Furthermore, it is faster and more convenient than the Kriging to generate. However, RBF is deficient in that the appearance of a metamodel varies significantly with the type of the basis function and its internal parameters [13]. In addition, this method does not provide a statistical

Table 1. Commonly used radial basis functions.

Name	Radial Function $r = \|\mathrm{x}\text{-}\mathrm{x}_i\|_2$
Linear	$\varphi(r)=cr$
Cubic	$\varphi(r)=(r+c)^3$
Thin plate spline	$\varphi(r)=r^2\log(cr^2)$
Gaussian	$\varphi(r)=\exp(-cr^2)$
Multiquadratic	$\varphi(r)=(r^2+c^2)^{1/2}$

prediction error as the Kriging technique [10] does. In this paper, a linear basis function is used with the fixed parameter, c=1.

2.2 Existing sequential sampling methods

2.2.1 Entropy approach

This approach defines entropy, a measure of the disorder in the universe, using a determinant of the correlation function representing the correlation between sampling points, and then maximizes the defined entropy [8]. The approach uses the Kriging model based on the Bayesian theory and an existing sample set $\mathbf{X}_P(\mathbf{x}_{P1}, \mathbf{x}_{P2},\ldots, \mathbf{x}_{P\ell})$, and selects a new sample set $\mathbf{X}_C(\mathbf{x}_{C1}, \mathbf{x}_{C2},\ldots, \mathbf{x}_{Cm})$ with the maximum amount of information.

$$\max_{\mathbf{x}_C} \left|\mathbf{R}_A\right| \times \left|\mathbf{J}^T \mathbf{R}_A^{-1} \mathbf{J}\right| \tag{4}$$

where, $|\mathbf{R}_A|$ is the determinant of the correlation function for $\mathbf{X}_A = \mathbf{X}_C \cup \mathbf{X}_P$, a sample set which consists of ℓ existing sample points and m new sample points, and $\mathbf{J}$ is a vector ($\mathbf{J}^T = \{1,\ldots,1\}_{1\times(\ell+m)}$) which consists of ($\ell$+$m$) elements of 1. The correlation coefficients θ_k (k=1,…,n_{dv}) in $\mathbf{R}_A$ are the same as the ones in the correlation function of Kriging model given by Eq. (2).

2.2.2 MSE approach

This approach is designed to improve the accuracy of a metamodel by adding only one sampling point at the location where the greatest error is expected to happen. The error measure is defined as the mean square error (MSE) which is a statistical prediction error from the Kriging model. The mathematical statement of this approach is given by Eqs. (5) and (6).

$$\max_{\mathbf{x}_C} MSE(\mathbf{x}_c) \tag{5}$$

where,

$$MSE(\mathbf{x}_C) = \sigma^2 \left(1 - \mathbf{r}^T \mathbf{R}^{-1} \mathbf{r} + \frac{\left(1 - \mathbf{J}^T \mathbf{R}^{-1} \mathbf{r}\right)^2}{\mathbf{J}^T \mathbf{R}^{-1} \mathbf{J}}\right). \tag{6}$$

This approach is a special case of the entropy approach, and it is identical to the entropy approach when it picks only one sampling point at each iteration [10].

2.2.3 IMSE approach

Introduced by Sacks, this approach selects a new sample set $\mathbf{X}_C$ that provides the least integrated mean square error (IMSE) by using the Kriging metamodel and an existing sample set $\mathbf{X}_P$ [6].

$$\min_{\mathbf{x}_C} \int MSE(\mathbf{x}) d\mathbf{x} \tag{7}$$

where,

$$MSE(\mathbf{x}) = \sigma^2 \left(1 - \mathbf{r}_A(\mathbf{x})^T \mathbf{R}_A^{-1} \mathbf{r}_A(\mathbf{x}) + \frac{\left(1 - \mathbf{J}^T \mathbf{R}_A^{-1} \mathbf{r}_A(\mathbf{x})\right)^2}{\mathbf{J}^T \mathbf{R}_A^{-1} \mathbf{J}}\right). \tag{8}$$

In the case of picking only one new sample point, the difference between the IMSE approach and the MSE approach is that the IMSE approach applies the average MSE to the entire design space. Furthermore, the MSE approach uses only the existing sample set $\mathbf{X}_P$ to compose the MSE, while the IMSE uses both $\mathbf{X}_C$ and $\mathbf{X}_P$.

2.2.4 Maximin distance approach

In the case of adding m new sample sets $\mathbf{X}_C$ to ℓ existing samples sets $\mathbf{X}_P$, the maximin distance approach selects a new sample set that maximizes the minimum distance between two sampling points in $\mathbf{X}_A = \mathbf{X}_C \cup \mathbf{X}_P$ [7].

$$\max_{\mathbf{x}_C} \left[\min_{1\le i\le m, 1\le j\le l+m}^{\mathbf{x}_{Ci} \ne \mathbf{x}_{Aj}} \left(d\left(\mathbf{x}_{Ci}, \mathbf{x}_{Aj}\right)\right)\right] \tag{9}$$

This approach uses only location information of the existing sample points to select the new sample points, which leads to a shortcoming of not being able to account for the response of the model.

2.2.5 Cross-validation approach

The MSE and IMSE approach are restricted within the Kriging model. And, the entropy and maximin distance approach cannot account for the response characteristics of the model (i.e., use only location information of sample points). The cross-validation approach, however, is one of the sequential sampling methods that has no restriction on using metamodeling techniques and accounting for the response characteristics of the model. The cross-validation ap-

proach validates the accuracy of a metamodel by constructing a metamodel while sequentially eliminating one or more existing sample points and then comparing the difference of the response of the metamodel over the entire existing sample points. This approach has a great advantage in that it does not require extra sampling points to measure the accuracy of the metamodel.

The prediction error can be calculated by Eq. (10) using the leave one-out cross-validation, the most widely used cross-validation approach which can generate a metamodel over a sample point set with one sample point excluded.

$$e(\mathbf{x}) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\hat{y}_{-i}(\mathbf{x}) - \hat{y}(\mathbf{x})\right)^2} \tag{10}$$

Where, N is the total number of sampling points, $\hat{y}(\mathbf{x})$ is the response of the metamodel which is generated over the entire existing sample set $\mathbf{X}_P$. $\hat{y}_{-i}(\mathbf{x})$ is the response of the metamodel which is generated over a set of sample points with the i th sample point excluded out of N sample points. The method selects a new sample point $\mathbf{x}$ with the greatest prediction error calculated by Eq. (10).

However, the sequential sampling based on Eq. (10) has a tendency that the new sampling point is very close to the existing sampling point $\mathbf{x}_{Pi}$, ending up with crowded new sample points near existing sample points. To prevent such a phenomenon from happening, Jin [10] modified Eq. (10) and suggested a method that can account for the distance between the new and existing sample points, and the modified Eq. is given by Eq. (11).

$$\max_{\mathbf{x}_C}\left[e(\mathbf{x}_C) * \min_i\left(d\left(\mathbf{x}_C, \mathbf{x}_{Pi}\right)\right)\right] \tag{11}$$

3. Construction of the radial basis function based on a sequential sampling approach using the cross-validation method

3.1 Defects of the existing cross-validation approach

A problem of Jin's cross-validation approach arises when the first metamodel (which is generated by using one-stage sampling approach) is not sufficiently accurate. If one calculates the prediction error with the response of the metamodel, which is constructed using insufficient sample points, Eq. (11) will lead the new sample point to a wrong location. Therefore, the sample points are probably wasted due to being placed in the wrong location. As a result, the resulting metamodel may have a lower accuracy rate even when the metamodel is generated by a one-stage approach which selects all sample points at once. Thus, the sequential sampling method accounting for the response characteristics of a metamodel only can be used when the metamodel possesses appropriate accuracy.

3.2 Proposed sequential sampling approach

The defects of Jin's approach can be overcome by modifying Eq. (11), resulting in an improved approach defined by the Eq. (12).

$$\max_{\mathbf{x}_C}\left[w_1 \times \frac{e(\mathbf{x}_C)}{\max\left[e(\mathbf{x}_{test})\right]} + w_2 \times \frac{2 \times \min\left(\mathbf{x}_C, \mathbf{x}_{Pi}\right)}{\min_{i \neq j}\left(\mathbf{x}_{Pi}, \mathbf{x}_{Pj}\right)}\right] \tag{12}$$

The reason for dividing the prediction error term by $\max[e(\mathbf{x}_{test})]$ is to normalize the prediction error to make its maximum and minimum as 1 and 0, respectively. For the same reason, the term representing the distance between points is normalized by being divided by $\frac{1}{2} \times \min_{i \neq j}\left(\mathbf{x}_{Pi}, \mathbf{x}_{Pj}\right)$. Since the two terms are normalized, the method is not sensitive to these scales

Thus, a logical and efficient sequential sampling approach can be proposed: first, assign 0 to the weight w_1 of the prediction error term for the inaccurate metamodels so that the maximin distance approach is used alone, and then increase the weight of the prediction error for metamodels that appear to be sufficiently accurate.

The algorithm of the proposed approach is explained below:

- Step 1: Set k, the number of iterations, to 1. Then, set w_1 (the weight of prediction error term) to 0, w_2 (the weight of minimum distance term) to 1. Use the Latin hypercube sampling method to generate the initial sample set $\mathbf{X}_P$, and perform an analysis over $\mathbf{X}_P$.
- Step 2: Use Eq. (10) to calculate the cross-validation error at the test points, and then find the greatest prediction error. Find the shortest distance between the existing sampling points $\mathbf{x}_{Pi}$ and $\mathbf{x}_{Pj}$ ($i \neq j$).

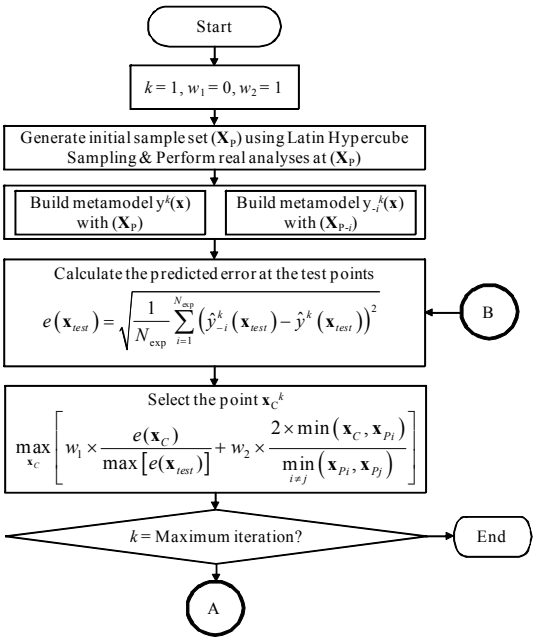

Fig. 1. Algorithm of the proposed approach.

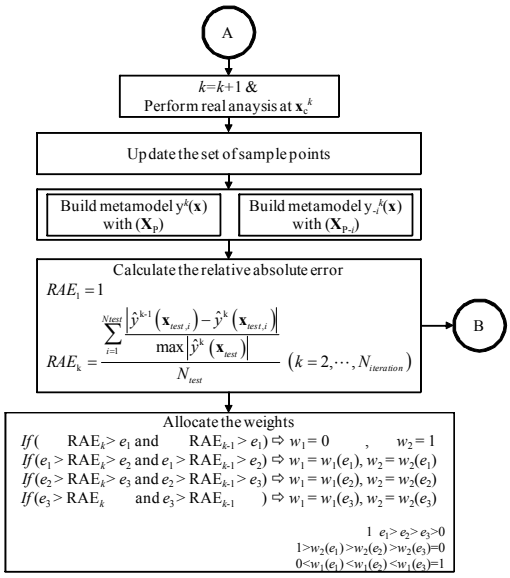

Fig. 2. Algorithm of the proposed approach.

- Step 3: Use the greatest prediction error and the shortest distance between the existing sampling points $\mathbf{X}_P$ found in Step 2 to establish Eq. (12), and then use global optimization to select a new sample point $\mathbf{x}_C$.
- Step 4: If the number of iterations k reaches the designer-specified value, then stop the process; otherwise proceed to the next step.
- Step 5: Perform analysis at $\mathbf{x}_C$ and set k=k+1. Update the existing sample set $\mathbf{X}_P$ by adding the new sample point $\mathbf{x}_C$ to $\mathbf{X}_P$.
- Step 6: Assign weights w_1 and w_2 based on the accuracy of the metamodel, and go back to Step 2.

The relative absolute error (RAE) value is identified as a measure of accuracy for the metamodels, and the error between the metamodels generated from the two successive iterations can be calculated by Eq. (13):

$$RAE_k = \frac{\sum_{i=1}^{Ntest}\left|\hat{y}^{k-1}(\mathbf{x}_{test,i}) - \hat{y}^k(\mathbf{x}_{test,i})\right|}{\max\left|\hat{y}^k(\mathbf{x}_{test})\right|} \Big/ N_{test} \quad (k = 1, \cdots, N_{iteration}) \tag{13}$$

where, N_{test} is the total number of sample points, $\hat{y}^k$ is the metamodel constructed at the k th iteration. When RAE_k resides within a range of 'sufficient value', a large value is assigned to the weight w_1 of the prediction error term that uses the response of the metamodel.

Here, because *RAE* is the accuracy measure which uses the information of the metamodel only, it shows instable tendency. To see these characteristics, *RAE* was compared with *RMSE* (which uses the information of actual model) according to the change of the number of sample points (from 8 to 50). Fig. 3 and Table 2 show the test functions used in this study. The maximin distance approach as a sequential sampling approach and the radial basis function based on the linear basis function as a metamodeling technique are used in these cases.

Fig. 4 to Fig. 7 depict the results of *RAE* and *RMSE* calculated for each function with respect to the number of sample points. It can be observed from the trend of the *RAE* that the error converges to 0 as iteration repeats, while it has peaks different from the uniform convergence of *RMSE*.

To make the algorithm be robust and insensitive to the peak values, it accounts for both RAE_k and RAE_{k-1} not only RAE_k. Namely, it increases the weight of the prediction error terms only when the *RAE* is less than a 'sufficient value' after two consecutive iterations. Where, the 'sufficient value' is defined as an infinitesimal positive number with the size of $1 \gg \varepsilon_1 > \varepsilon_2 > \varepsilon_3 > 0$. In addition, if the conditions of $RAE_{k-1} < \varepsilon_1$ and $RAE_k < \varepsilon_1$ are satisfied, w_1 is defined as $w_1(\varepsilon_1)$.

Table 2. Test function.

Name	Function
Branin	$y=\left[x_2-5.1\times\left(\frac{x_1}{2\pi}\right)^2+\frac{5x_1}{\pi}-6\right]^2$ $+10\times\left(1-\frac{1}{8\pi}\right)\times\cos(x_1)+10$ $x_1\in[-5,10],\quad x_2\in[0,15]$
Waving	$y=2+0.01\left(x_2-x_1^2\right)^2+\left(1-x_1\right)^2+2\left(2-x_2\right)^2$ $+7\sin\left(0.5x_1\right)\sin\left(0.7x_1x_2\right)$ $x_1,x_2\in[0,5]$
Waving-linear	$y=\cos\left(6\left(x_1-0.5\right)\right)+3.1\left(\left\|x_1-0.7\right\|\right)+2\left(x_1-0.5\right)$ $+\sin\left(\frac{1}{\left\|x_1-0.5\right\|+0.31}\right)+0.5x_2$ $x_1,x_2\in[0,1]$
Goldstein and Price	$y=\left[1+\left(x_1+x_2+1\right)^2\begin{pmatrix}19-14x_1+3x_1^2\\-14x_2+6x_1x_2+3x_2^2\end{pmatrix}\right]^2\times$ $\left[30+\left(2x_1-3x_2\right)^2\times\begin{pmatrix}18-32x_1+12x_1^2+48x_2\\-36x_1x_2+27x_2^2\end{pmatrix}\right]$ $x_1,x_2\in[-5,2]$

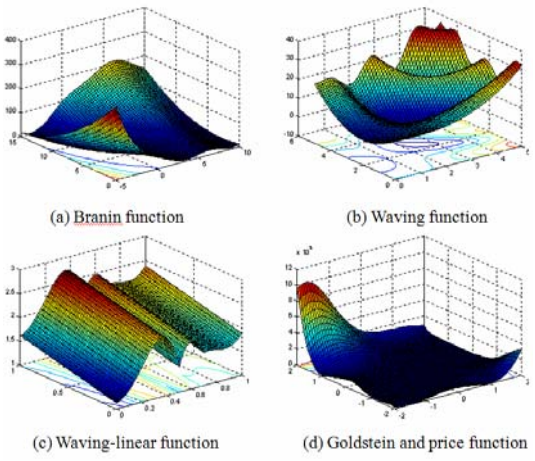

Fig. 3. Test function.

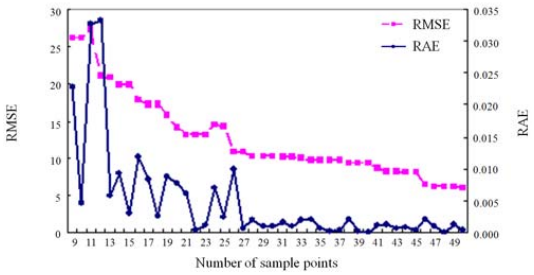

Fig. 4. RMSE & RAE of Branin function.

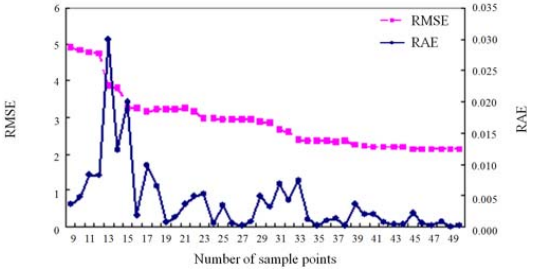

Fig. 5. RMSE & RAE of Waving function.

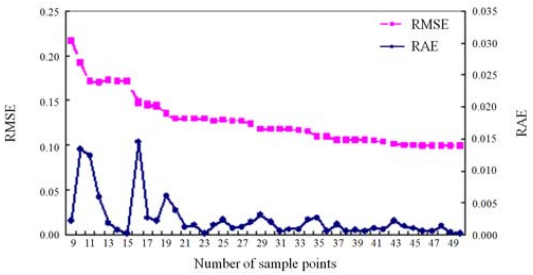

Fig. 6. RMSE & RAE of Waving-linear function.

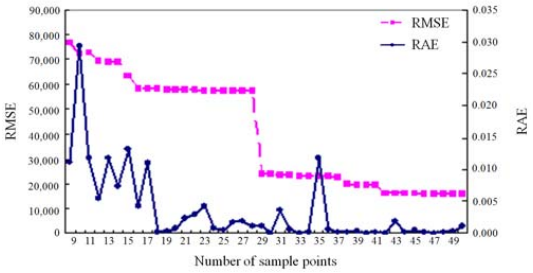

Fig. 7. RMSE & RAE of Goldstein and price function.

3.3 Determination of the parameters

In the proposed approach, there are parameters that need to be specified by a designer and they are ε_1, ε_2, ε_3, $w_1(\varepsilon_1)$, $w_2(\varepsilon_1)$, $w_1(\varepsilon_2)$, $w_2(\varepsilon_2)$, $w_1(\varepsilon_3)$, $w_2(\varepsilon_3)$. In other words, the designer has to determine how small the *RAE* should be for efficiently defining an accurate metamodel, and how the weights should be assigned for the terms in Eq. (11). If the summation of w_1 and w_2 is known as 1, the parameters needed to be determined will be ε_1, ε_2, ε_3, $w_1(\varepsilon_1)$, $w_1(\varepsilon_2)$, $w_1(\varepsilon_3)$.

Fig. 4 to Fig. 7 depict that, generally, the *RAE* is less than 0.002 for the cases that converge in a very stable manner. In addition, the *RAE* never exceeds 0.035 for any case. Based on these findings, after several trial-and-errors are performed, the parameters are determined and listed in Table 3:

Table 3. The best parameters based on the trial & errors.

	ε	w_1	w_2
Initial		0	1
1st criterion	0.019	0.2	0.8
2nd criterion	0.07	0.5	0.5
3rd criterion	0.001	0.8	0.2

4. Test problems

4.1 Problem definition

To compare and analyze the accuracy of the metamodel created by using the proposed sequential sampling approach, four of the two-variable mathematical function problems shown in Fig. 3 and Table 2 that Jin [10] used are chosen as proof of implementation in this study. The functions used in the test are all strong non-linear functions: (a)Branin function, (b)Waving function, (c)Waving-linear function and (d)Goldstein and Price function.

4.2 Test scheme

In this study, the same test scheme as the one presented in [10] is used: the number of the initial and the final sample points are 8 and 24, respectively, for all 2-variable problems. Instead of using the entropy criterion in the optimal Latin hypercube sampling (OLHS) [14] method, the maximin distance criterion is used in this study to generate the initial sample points. When generating sample points by using OLHS, there exists randomness. Because the accuracy of a metamodel is very sensitive to the sample points, in order to eliminate the effect of randomly used sample points existing in the initial sample points, 10 repeat tests using the average value are conducted.

To compare the accuracy of the metamodels, additional 800 test points generated by the MCS method are utilized. As a measure of accuracy, the root mean squared error (RMSE) is used to evaluate the prediction performance of the global functions, given by Eq. (14).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N_{test}} \left(\hat{y}(\mathbf{x}_{test,i}) - y(\mathbf{x}_{test,i}) \right)^2}{N_{test}}} \tag{14}$$

where, N_{test} is the number of test points, y is the response of an actual function and $\hat{y}$ is the response of a metamodel.

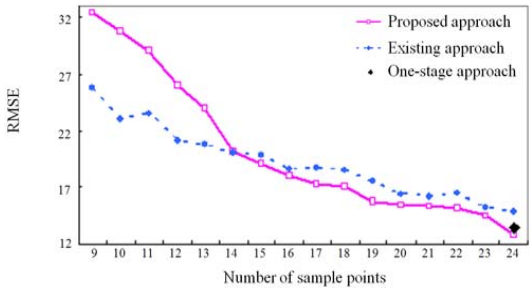

Fig. 8. RMSE history of Branin function.

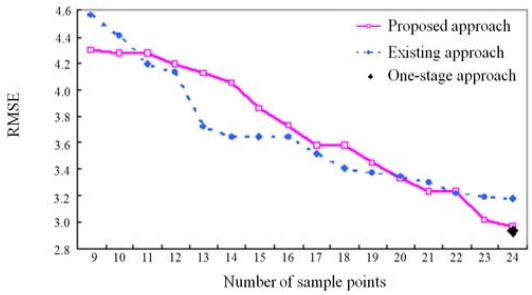

Fig. 9. RMSE history of Waving function.

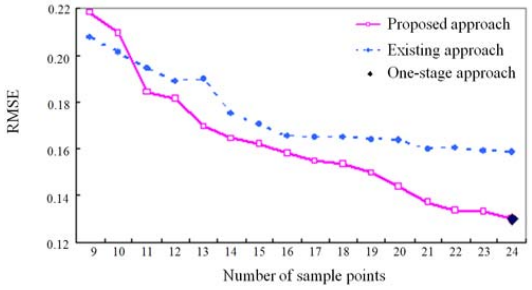

Fig. 10. RMSE history of Waving-linear function.

To evaluate the proposed sequential sampling approach, the results obtained from the 'one-stage' method using the OLHS technique at the final sample points and the results obtained from the existing sequential sampling approach [10] are compared to the results from proposed method.

4.3 Result of the test

Fig. 8 to Fig. 11 depict the RMSE of each function for the proposed approach in this work. Table 4 shows a comparison of the accuracy of the metamodels in terms of the RMSE over 24 sample points, which is the final metamodel in this test scheme.

Table 4. Comparison of the RMSE of the final metamodel.

Function Name	RMSE of the final metamodel			Improvement of the accuracy (%)	
	Proposed approach	Existing approach	One-stage	Proposed vs. Existing	Proposed vs. One-stage
Branin	12.86	14.90	13.50	***15.91***	***5.00***
Waving	2.97	3.17	2.93	***6.81***	***-1.30***
Waving-linear	0.13	0.16	0.13	***21.84***	***0.04***
Goldstein and price	27358.03	36012.44	45540.45	***31.63***	***66.46***

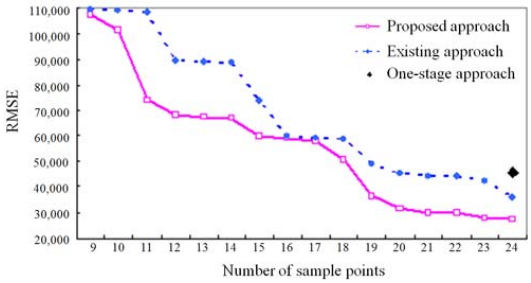

Fig. 11. RMSE history of Goldstein and price function.

The results reveal that the proposed approach in this study can improve the accuracy of a metamodel by 6.81% to 31.63%, that is, 19.05% on average, as compared to the existing cross validation approach. Compared to the "one-stage" approach in terms of the RMSE, although the proposed approach shows –1.30% worse in accuracy for the Waving function, it improves the accuracy by 0.04% to 66.46%, a 17.55% in average, for the other functions. The proposed approach and the "one-stage" approach have similar accuracy for the Waving function and Waving-linear function that have strong nonlinearity over the entire design space. However, for the Goldstein and Price function that has locally strong nonlinearity, the proposed approach exhibits abrupt dramatic improvement of 66.46% in accuracy.

5. Conclusions and future works

This study proposed a sequential sampling approach that can overcome the defects of the existing cross-validation approach. The capabilities of the approach were demonstrated by various mathematical testing problems. Their results revealed that the proposed approach improved the accuracy by 19.05% and 17.55% on average over the existing "cross-validation" approach and "one-stage" approach, respectively. Although it can be concluded that the proposed approach constructs a more accurate metamodel than the existing cross-validation approach, it is not prudent to claim that this proposed approach is better than the "one-stage" approach since three out of four test problems did not show significant improvement in accuracy when compared to the "one-stage" approach.

The accuracy of the metamodel is not the only measure which is used to compare the sequential sampling approach and the "one-stage" approach. If the two approaches have the same accuracy for a specified problem, the sequential sampling approach would still be the better choice because in the sequential sampling approach the changes in accuracy can be seen, which will highly facilitate the determination of the termination criteria for the problem under consideration. The existing cross-validation approach generally has a lower accuracy rate than the "one-stage" approach, which is often a reason why designers hesitate to use it as the preferred sampling approach. However, it is clear that the proposed approach is the better choice over the "one-stage" approach because it shows similar or higher accuracy and provides a trend of changes in accuracy of a metamodel.

Considering the approach was applied to only four two-variable problems, follow-on research should be conducted when implementing the proposed approach to more various problems. In addition, the research on the parameters that the designers need to specify is another area to study in depth. Finally, in this study, although the proposed sequential sampling method focuses on the global metamodeling, the research on the sequential sampling method for the Sequential Approximate Optimization (SAO) is needed.

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