A Novel Adaptive Dynamic Taylor Kriging and Its Application to Optimal Design of Electromagnetic Devices

Bin Xia[1], Tae-Woong Lee[1], Kyung Choi[2], and Chang-Seop Koh[1], *Senior Member, IEEE*

[1]College of ECE, Chungbuk National University, Chungbuk, 361-763, Korea, tiandixiabin@chungbuk.ac.kr
[2]School of Electrical and Electronics Engineering, Kangwon National University, Kwangwon 200-701, Korea

An adaptive dynamic Taylor Kriging (ADTK) is developed and combined with the particle swarm optimization algorithm to get a numerically efficient optimization strategy. In the ADTK, the optimal basis function set is dynamically selected so that the generated surrogate model may have better accuracy. An adaptive sampling method about how many sampling points are required for a specific fitting accuracy is proposed. The proposed approach was tested on the analytic function and the TEAM 25 problem.

***Index Terms*— Benchmark problem, fitting accuracy, Kriging surrogate model, TEAM 25 problems.**

I. Introduction

HEURISTIC OPTIMIZATION algorithms such as particle swarm optimization (PSO) and differential evolution are widely being used in the optimal design of electromagnetic devices. However, they in general require a large number of objective function evaluations, and this often limits their application to engineering problems through direct combination with finite element analysis (FEA) [1]-[2]. As a solution to this, Kriging models such as ordinary Kriging, universal Kriging and Taylor Kriging have been developed to construct a surrogate objective function from the objective function values calculated on limited number of sampling points.

The fitting accuracy (or prediction accuracy) of the Kriging models, however, strongly depends on the problem as well as the number and locations of sampling points. The problem dependency of the Kriging models is very recently reported to be mitigated by introducing dynamic version of Kriging model which optimally selects its basis functions among its originally ones [3]. For the number and locations of the sampling points which guarantee a desired fitting accuracy, however, any reliable algorithm is not presented yet except that the more sampling points and the higher fitting accuracy.

In this paper, a novel adaptive dynamic Taylor Kriging is suggested for the application to optimal design of electromagnetic devices by combining dynamic Taylor Kriging with an adaptive sampling method. Furthermore, a reliable algorithm for the decision of minimal required number of sampling points and estimation of fitting error are proposed. Through applications to an analytic function and TEAM 25, the validity of the developed algorithm is investigated.

II. Dynamic Taylor Kriging

For an arbitrary point **x** in design space, the dynamic Taylor Kriging (DTK) predicts a function value as follows:

$$Z^*(\mathbf{x}) = \sum_{i=1}^{N} \lambda_i(\mathbf{x}) Z(\mathbf{x}_i) \tag{1}$$

where N is the number of sampling points, $Z(\mathbf{x}_i)$ is the objective function value at the point $\mathbf{x}_i$ and the weighting coefficient $\lambda_i(\mathbf{x})$ is found from the following equations:

$$\sum_{i=1}^{N} \lambda_i(\mathbf{x}) b_k(\mathbf{x}_i) = b_k(\mathbf{x}), \quad k = 0,1,\cdots,K \tag{2-a}$$

$$\begin{aligned}&\sum_{i=1}^{N} \lambda_i Cov[Z(\mathbf{x}_i), Z(\mathbf{x}_j)] + \sum_{k=0}^{K} \delta_k b_k(\mathbf{x}_j) \\ &\quad = Cov[Z(\mathbf{x}), Z(\mathbf{x}_j)], \quad j = 1,\cdots,N\end{aligned} \tag{2-b}$$

where K is the number of basis functions, $Cov(\cdot,\cdot)$ is the Gaussian covariance function, δ is Lagrange multiplier, and the basis function $b_k(\mathbf{x})$ is defined as follows [4]:

$$b_k(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_0)^k \tag{3}$$

where $\mathbf{x}_0$ is the mean value of all sampling points.

In constrast to other Kriging models such as ordinary Kring, universal Kriging and Taylor Kriging, the DTK optimally selects its basis functions to minimize its fitting error [3]. In this paper, the set of optimal basis functions is found by solving the following equation using an improved B-PSO algorithm proposed in [5]:

$$\text{minimize} \quad Q(\mathbf{C}_p) = \frac{1}{NTS} \sum_{i=1}^{NTS} d(\mathbf{x}_i)\Big|_{\mathbf{C}_p} \tag{4}$$

where $\mathbf{C}_p$ is an arbitrary combination of basis functions, $\mathbf{x}_i$ (i=1, 2, ··; NTS) is the test points, and $d(\cdot)$ is the bandwidth of the 1-α level prediction interval which is defined as:

$$\begin{aligned}&d(\mathbf{x}) = 2Z_{1-\alpha/2}\sigma_{\mathrm{p}}^2(\mathbf{x}) \\ &\sigma_{\mathrm{p}}^2(\mathbf{x}) = \sigma^2[1 + \boldsymbol{\lambda}^T(\mathbf{x})\mathbf{R}\boldsymbol{\lambda}(\mathbf{x}) - 2\boldsymbol{\lambda}^T(\mathbf{x})\mathbf{r}(\mathbf{x})]\end{aligned} \tag{5}$$

where $Z_{1-\alpha/2}$ is the α-level quantile of the standard normal distribution (α is set to 1.95 in this paper), **r(x)** is correlation vector, **R** is the Gaussian correlation matrix and σ^2 is the variance of the fitting error.

III. Adaptive Dynamic Taylor Kriging

A. Fitting Error Estimation

After a given number of initial sampling points are generated based on their geometric distribution by using Latin hypercube design (LHD), a Kriging surrogate model bounds its fitting error as follows:

$$\left| Z(\mathbf{x}) - Z^*(\mathbf{x}) \right| \le d(\mathbf{x})/2 = \mathrm{E}_{fitting}(\mathbf{x}) \tag{6}$$

where $Z^*(\mathbf{x})$ and $Z(\mathbf{x})$ are predicted value from a surrogate model and true function value at **x**, respectively.

B. Adaptive Insertion of Sampling Point

If the fitting error is not small enough, new sampling points are selected adaptively among the test points, $\mathbf{X}_{\text{test}}$, based on the following rule using (5):

$$\mathbf{X}_{\text{new}} = \left\{ \mathbf{x} \middle| d(\mathbf{x}) > \varepsilon, \mathbf{x} \in \mathbf{X}_{\text{test}} \right\} \tag{7}$$

where the tolerance ε is, in this paper, set to 10^{-4}. The smaller the tolerance is taken, the smaller the fitting error is expected.

C. Termination Criterion

The adaptive sampling insertion may be repeated until the termination criterions Avg($\mathbf{X}_S{}^k$) and Max($\mathbf{X}_S{}^k$) are both satisfied. The termination criterion can be defined as follows:

$$\text{Avg}(\mathbf{X}_S^k) = \sqrt{\sum_{i=1}^{NTS} \left(\text{E}_{fitting}(\mathbf{x}_i)\right)^2 \Big/ NTS} < 10^{-3} \tag{8-a}$$

$$\text{Max}(\mathbf{X}_S^k) = \max_{1 \le i \le NTS} \text{E}_{fitting}(\mathbf{x}_i) < 10^{-3} \tag{8-b}$$

where $\mathbf{X}_S{}^k$ is the set of sampling points at k-th iteration, $\text{E}_{fitting}$ is defined from (6), and NTS is the number of testing points.

IV. Applications to Optimal Design

In order to investigate and compare the fitting accuracy of the surrogate models, an analytic test function is selected as:

$$\begin{aligned} \text{maximize} \quad & \text{F} = 3(1-x_1)^2 \exp\left[-x_1^2 - (x_2+1)^2\right] \\ & -10\left(\frac{x_1}{5} - x_1^3 - x_2^5\right)\exp\left(-x_1^2 - x_2^2\right) \\ & -\frac{1}{3}\exp\left[-(x_1+1)^2 - x_2^2\right] \\ \text{subject to} \quad & -3 \le x_1, x_2 \le 3 \end{aligned} \tag{9}$$

and the root mean square error (RMSE) and the maximal error are defined as follows:

$$\text{RMSE} = \sqrt{\sum_{i=1}^{NTS} \left[Z^*(\mathbf{x}_i) - Z(\mathbf{x}_i)\right]^2 \Big/ NTS} \tag{10}$$

$$\text{Maxerror} = \max_{1 \le i \le NTS} \left| Z^*(\mathbf{x}_i) - Z(\mathbf{x}_i) \right| \tag{11}$$

where the number of test points NTS is set to 1600.

Fig. 1 shows the behavior of the average fitting error Avg($\mathbf{X}_S$) together with the RMSE for the adaptive dynamic Taylor Kriging (ADTK) model, and Fig. 2 shows the behavior of the maximal fitting error Max($\mathbf{X}_S$) together with the maximal error for the ADTK model, where it is found that Avg($\mathbf{X}_S$) and Max($\mathbf{X}_S$) are both good metrics for the real fitting error. Firstly, the initial 25 sampling points are generated by using LHD, and the additional sampling points are adaptively inserted to have totally 70 sampling points. Table I compares the optimization results obtained by using the PSO algorithm combined with the ADTK model (ADTK-PSO) and directly PSO algorithm. The adaptive sampling method can yield the enough sampling points for reducing computing time. Therefore, it shows the DTK model with adaptive sampling method can generate an accurate surrogate model very efficiently.

In the version of full paper, the developed algorithm will be applied to TEAM 25, a strongly non-linear problem, and its effectiveness will be demonstrated.

Algorithm: *Adaptive Dynamic Taylor Kriging*

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1. ***Initial sampling and test points***
   - Generate N sampling points using Latin hypercube design, and prepare NTS test points which are uniformly distributed.
   - Set the tolerance ε for $d(\mathbf{x})$.
2. ***Construct DTK***
   - For all sampling points, calculate the objective function and constraint function values by using finite element analysis.
   - Find an optimal basis functions by using the B-PSO algorithm, and construct the DTK model.
   - Calculate $d(\mathbf{x})$ for all NTS test points, and if Avg($\mathbf{X}_S$) $\le 10^{-3}$ and Max($\mathbf{X}_S$) $\le 10^{-3}$, then terminate.
3. ***Adaptive sampling***
   - Select N_{step} test points in the order of $d(\mathbf{x})$, and insert them into the set of sampling points.
   - Go to Step 2.

V. References

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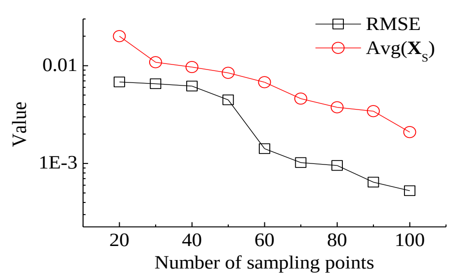

Fig. 1 Behavior of average of fitting error in ADTK model

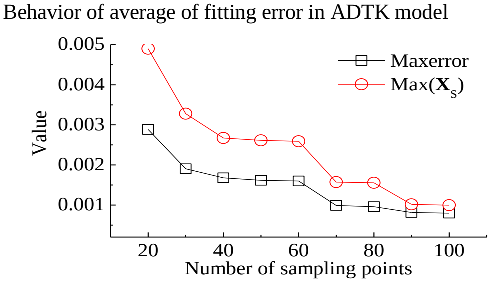

Fig. 2 Behavior of maximal fitting error in ADTK model

TABLE I
OPTIMIZATION RESULTS FOR ANALYTIC FUNCTION

Method	Optimum point	Objective value	Calls
ADTK-PSO	[-0.0062, 1.5798]	8.1058	70
PSO	[-0.0061, 1.5808]	8.1061	3000