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Stabilization of parameter estimation for Kriging-based approximation with empirical semivariogram

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ABSTRACT

This paper discusses stabilization of an optimization procedure to determine an appropriate semivariogram parameter using the empirical semivariogram for Kriging-based approximation. From a viewpoint of a computational cost for constructing a surrogate model, a semivariogram fitting approach using the empirical semivariogram can be usable for the parameter estimation of a semivariogram function. However, instability of the optimization procedure for determination of the semivariogram parameter may be observed in some cases and it causes to generate an invalid surrogate model.
For this problem, a simple technique for stabilization of the optimization for the parameter determination is proposed in this paper. The proposed approach employs a normalization technique of input data with respect to values of variables and an objective function. The proposed method is applied to some numerical examples, and the numerical results illustrate validity and effectiveness of the proposed method.

1. Introduction

The Kriging method has been widely used for approximation of a response function, and it is used for approximate optimization in an engineering field such as structural optimization or a part of an optimization strategy in recent works [1–5]. Approximation with noisy or inaccurate data set has been attempted using the Kriging-based approach [6–11], and it will be helpful for approximate optimization in an engineering field. Also, Kriging approximation is used for some numerical analyses in mechanics [12–14].

A surrogate model using the Kriging method can be constructed using some kinds of semivariogram parameter identification such as the most likelihood estimator (MLE) [15] or fitting semivariogram function [16]. The latter approach uses a primitive semivariogram function, which is called as the empirical semivariogram, as a target function of the parameter identification. This approach is called as “empirical semivariogram-based approach” in this paper.

Simpson et al. reported that the MLE-based Kriging method requires a high computational cost for constructing a surrogate model [17]. On the other hand, the empirical semivariogram-based approach enables to reduce the computational cost.

However, in using the empirical semivariogram-based approach, an inappropriate approximated result is sometimes observed. It is considered that this fact may be caused by instability of the optimization process in the parameter identification, and a reason of the instability or a way for improvement of the stability should be discussed.

For this problem, a reason of the instability is discussed from a viewpoint of the semivariogram parameter determination process for the Kriging-based approximation in this paper. At first, outline of the Kriging method is introduced. Next, instability of the parameter estimation and the proposed method for improving the parameter determination process are discussed. Some numerical examples illustrate validity and effectiveness of the proposed method.

2. Kriging-based approximation

In this paper, the ordinary Kriging method is used for approximation. The empirical semivariogram-based approach is used for determination of semivariogram parameters. The Kriging method is a spatial prediction method that minimizes variance of the prediction error. A linear predictor of $\hat{Z}(\boldsymbol{s}_0)$ can be computed as

$$\hat{Z}(s_0) = w(s_0)^T \boldsymbol{Z} \tag{1}$$

where $\boldsymbol{w} = \{w_1, w_2, \cdots, w_n\}^T$ is a weighting coefficient vector, $\boldsymbol{Z} = \{Z(\boldsymbol{s}_1), Z(\boldsymbol{s}_2), \cdots, Z(\boldsymbol{s}_n)\}^T$ is an observed value vector which is obtained as sampling values at the nth known locations $\boldsymbol{s}_1$, $\boldsymbol{s}_2$ $\cdots$, $\boldsymbol{s}_n$ in a solution space $\boldsymbol{S}$, $\hat{Z}(\boldsymbol{s}_0)$, which shows an estimated value of $Z(\boldsymbol{s}_0)$ at $\boldsymbol{s}_0 \in \boldsymbol{S}$, which is the point where we want to estimate the value of the function. The estimated value $\hat{Z}(\boldsymbol{s}_0)$ can be calculated by the sum of the weighted sampling values at each location.

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The weighting coefficient w can be calculated by Eq. (2).

$$w = \boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma}_0 + \left(\frac{1-\boldsymbol{1}^T\boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma}_0}{\boldsymbol{1}^T\boldsymbol{\Gamma}^{-1}\boldsymbol{1}}\right)\boldsymbol{\Gamma}^{-1}\boldsymbol{1} \tag{2}$$

where $\boldsymbol{1}=\{1, 1, \cdots, 1\}^T$. We can use a cheaper form for the estimation instead of Eqs. (1) and (2) as

$$\hat{Z}(s_0) = \boldsymbol{\gamma}_0^T g_F + \frac{1}{b}\left(1-\left(\boldsymbol{\gamma}_0^T g_1\right)\right)\boldsymbol{1}^T g_F \tag{2$'$}$$

where $\mathbf{g}_F=\boldsymbol{\Gamma}^{-1}\boldsymbol{Z}$, $\mathbf{g}_1=\boldsymbol{\Gamma}^{-1}\boldsymbol{1}$ and $b=\boldsymbol{1}^T\boldsymbol{\Gamma}^{-1}\boldsymbol{1}$. $\boldsymbol{\Gamma}$ and $\boldsymbol{\gamma}^*$ in Eq. (2) are a coefficient function matrix and vector, which are expressed as

$$\boldsymbol{\Gamma} = \left\{\gamma\left(s_i - s_j\right)\right\}_{ij} \tag{3}$$

$$\boldsymbol{\gamma}_0 = \{\gamma(s_1-s_0), \cdots, \gamma(s_n-s_0)\}^T \tag{4}$$

where γ is a semivariogram function. Several types of semivariogram, for example a sphere type or an exponential type, have been proposed. In this study, the Gaussian-type semivariogram model with the nugget effect, which is expressed by Eq. (5), is adopted.

$$\gamma(\boldsymbol{h}_i;\boldsymbol{\beta}) = \begin{cases} \beta_0 + \beta_1\left[1-\exp\left(-\left\{\frac{\|\boldsymbol{h}_i\|}{\beta_2}\right\}^2\right)\right] & : \|\boldsymbol{h}_i\| \neq 0 \\ 0 & : \|\boldsymbol{h}_i\| = 0 \end{cases} \tag{5}$$

where $\boldsymbol{h}$ is a vector, which is expressed by the difference between each observed location $\boldsymbol{s}_i$ and estimating location $\boldsymbol{s}$. β_0, $\beta_1 \geq 0$, $\beta_2 > 0$ are the model parameters. β_0 is called as the nugget effect, β_1 is the sill and β_2 is the range. Generally β_0 is not used for a set of accurate data.

In order to determine the parameter $\boldsymbol{\beta}$, the empirical-based approach is used in this study. It is assumed that an empirical semivariogram can be expressed as follows [18]:

$$\hat{\gamma}(\boldsymbol{h}) = \frac{1}{2|N_k|}\sum_{N_k}\left(Z(s_i)-Z(s_j)\right)^2 \tag{6}$$

where N_k is the number of samples in a data set that satisfies

$$|s_i - s_j| \in (R_{k-1}, R_k],\ 0<R_{k-1}<R_k \in \boldsymbol{R}^1. \tag{7}$$

To determine the parameter $\boldsymbol{\beta}$, Cressie's criterion (Cressie [19]), which is considered as a robust and efficient estimator for changes in the scale of data using this type of semivariogram, is used. The Cressie's weighted least squares criterion, which is to be minimized for determination of the optimum semivariogram parameters, can be written as

$$WLS(\boldsymbol{\beta}) = \sum_{k=1}^{K}\frac{|N_k|}{\gamma(\boldsymbol{h}_k,\boldsymbol{\beta})}\left(\hat{\gamma}(\boldsymbol{h}_k)-\gamma(\boldsymbol{h}_k,\boldsymbol{\beta})\right)^2. \tag{8}$$

3. Instability of semivariogram parameter estimation using the empirical semivariogram

In using the empirical semivariogram-based approach with the Cressie's criteria, a computational cost for determination of the semivariogram parameter will be cheaper than the most likelihood estimator (MLE) based approach. However, instability of the optimization process to determine a set of appropriate semivariogram parameters will be observed in some cases of using the empirical semivariogram-based approach. In this section, the instability of the parameter estimation and an estimated result using an invalid semivariogram parameter are introduced.

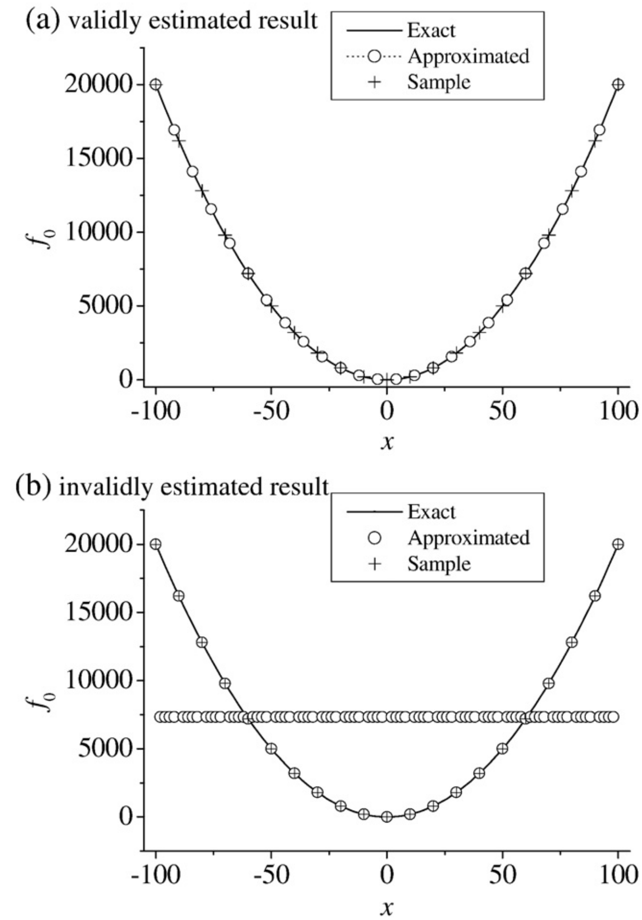

Fig. 1. An example of valid and invalid approximated results using the empirical semivariogram-based ordinary Kriging method.

As an example, the Kriging method is applied to construct a surrogate model for the following simple mathematical function.

$$f_0(x) = 2x^2\ (-100<x<100) \tag{9}$$

The exact surface, samples and validly estimated surface are illustrated in Fig. 1(a). If the parameter estimation process is successfully completed, an appropriate surrogate model can be obtained as shown in Fig. 1(a). However, instability of the parameter

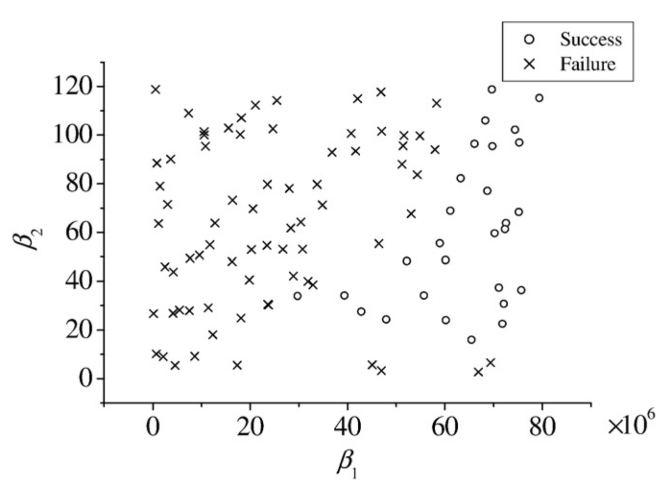

Fig. 2. Results of success or failure to obtain a valid approximation with using each set of semivariogram parameter as initial values.