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Extended Co-Kriging interpolation method based on multi-fidelity data

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ABSTRACT

The common issue of surrogate models is to make good use of sampling data. In theory, the higher the fidelity of sampling data provided, the more accurate the approximation model built. However, in practical engineering problems, high-fidelity data may be less available, and such data may also be computationally expensive. On the contrary, we often obtain low-fidelity data under certain simplifications. Although low-fidelity data is less accurate, such data still contains much information about the real system. So, combining both high and low multi-fidelity data in the construction of a surrogate model may lead to better representation of the physical phenomena. Co-Kriging is a method based on a two-level multi-fidelity data. In this work, a Co-Kriging method which expands the usual two-level to multi-level multi-fidelity is proposed to improve the approximation accuracy. In order to generate the different fidelity data, the POD model reduction is used with varying number of the basis vectors. Three numerical examples are tested to illustrate not only the feasibility and effectiveness of the proposed method but also the better accuracy when compared with Kriging and classical Co-Kriging.

1. Introduction

Many engineering optimization problems may be presented by partial differential equations. With advances in science, the major issue is managing computational effort (CPU time, memory, and interfacing) due to the cost of the high fidelity numerical simulations (finite elements, finite volumes, etc.) involved. In order to decrease the overall cost, reduced-order models are an economical and efficient option.

A wide range of approximation techniques [1,2] consists in replacing a complicated numerical model by a lower order meta-model, usually based on polynomial response surface methodology (RSM), kriging, least squares regression and moving least squares [3]. Surrogate functions and reduced order meta-models have also been used in the field of control systems to reduce the order of the overall transfer function [1]. Another popular physics-based meta-modeling technique [4] allows

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for benefiting in more extent from the full-field information provided by the numerical models [5]. It has been successfully applied to a number of areas such as flow modeling [6,7], optimal flow control [8], aerodynamics design optimization [9,10] or structural mechanics [11,12]. These approximated models have been constructed based on the accurate high-fidelity data samples only.

Kennedy proposed Co-Kriging method [13] considering not only high-fidelity data but also low-fidelity data. Similar to Kriging method [14], it is an interpolation technique based on statistical theory, and consists of a parametric linear regression model and a non-parametric stochastic process. Surrogate modeling based on Co-Kriging has received much attention during past decade. Forrester et al. [15] arranged its detailed description and analysis including the code resources of both Kriging and Co-Kriging models. The main theory is based on the Markov property. That means each level of fidelity only considered the influence of the nearest level information. The design space should satisfy the subset relationship and the smallest subset in the high-fidelity design space. Then, an efficient approach for sampling update for Co-Kriging has proposed by Elsayed [16] and successfully applied in the optimization of the cyclone separator geometry. Furthermore, a recursive Co-Kriging model is provided by Gratiet [17] and Gratiet and Garnier [18] to reduce the complexity of the model by building independent Kriging. In 2017, Parussini et al. [19] extended the recursive Co-Kriging to vector-valued fields and various types of covariances. Recently, laser beam welding process parameter optimization approach was discussed by Zhou et al. [20] with support vector regression constructing with two-level fidelity data: low fidelity computer simulations and high fidelity physical experiments. Wu and Murray [21] used Co-Kriging method to estimate population density in urban areas. In 2011, Co-Kriging of additive log-ratios was implemented to determined global grades of iron, silica and so on by Boezio et al. [22]. Han et al. [23] proposed a new Co-Kriging method for variable-fidelity surrogate modeling of aerodynamic data. Moreover, recent application of recursive Co-Kriging model was discussed by Singh et al. [24] with the scheme being demonstrated using triple-fidelity data obtained from physical experiments, CFD simulations and analytical models, respectively.

In this paper, we extend the usual two-level multi-fidelity model to a multi-level to improve the approximation accuracy. The other contribution of this work is to propose the strategy for constructing the multi-level multi-fidelity data based on POD models. Proper orthogonal decomposition (POD) (also known as Karhunen–Loeve expansions in signal analysis and pattern recognition [25], or the Principal Component Analysis in statistics [26], or the method of empirical orthogonal functions in geophysical fluid dynamics [27,28]) is a procedure for extracting a basis for model decomposition from an ensemble of snapshots. Based on the process constructed by POD [8], one can vary the basis size to obtain different fidelity snapshots used in Co-Kriging.

The paper is organized as follows: in Section 2, we present the simple procedure for the construction of general Co-Kriging. A new Co-Kriging model is described in details based on multiple levels of fidelity in Section 3. The verification of the feasibility and effectiveness of proposed method is discussed in Section 4 by means of three numerical experiments. The paper ends with conclusions and future goals.

2. General two-level multi-fidelity Co-Kriging

Co-Kriging is considered as a natural extension to the popular method of Kriging, but correlates multiple sets of data, and thus usually leads to a complex notation. To simplify the model, many researchers limit the data sets to two. With two levels [15], Co-Kriging approximates the high-fidelity model $\mathbf{y}_e(x)$ using the formula

$$\mathbf{y}_e(x) = \rho\mathbf{y}_c(x) + \mathbf{y}_d(x) \tag{2.1}$$

where $\mathbf{y}_c(x)$ denotes a Kriging model of a low-fidelity function and $\mathbf{y}_d(x)$ the difference between the low-fidelity function and a high-fidelity function. Assume two sets of data(high-fidelity and low-fidelity)be given. The high-fidelity model has n_e samples $(\mathbf{X}_e^{\mathrm{T}}, \mathbf{y}_e^{\mathrm{T}}) = ((x_e^{(1)}, y_e(x_e^{(1)})), \dots, x_e^{(n_e)}, y_e(x_e^{(n_e)})))$, and low-fidelity model has n_c samples $(\mathbf{X}_c^{\mathrm{T}}, \mathbf{y}_c^{\mathrm{T}}) = ((x_c^{(1)}, y_c(x_c^{(1)})), \dots, (x_c^{(n_c)}, y_c(x_c^{(n_c)})))$. In order to evaluate the unknown value y_e at point $x^{(n_e+1)}$,first we augment the observed data with the predicted value

$$\tilde{\mathbf{X}} = \left\{\mathbf{X}_c^{\mathrm{T}} \quad \mathbf{X}_e^{\mathrm{T}} \quad x^{(n_e+1)}\right\}^{\mathrm{T}}, \quad \tilde{\mathbf{y}} = \left\{\mathbf{y}_c^{\mathrm{T}} \quad \mathbf{y}_e^{\mathrm{T}} \quad y_e\left(x^{(n_e+1)}\right)\right\}, \tag{2.2}$$

Here each component of $\tilde{\mathbf{y}}$ is a normally distributed random variable with the same mean μ and variance σ^2 and $\mathbf{y} = \{\mathbf{y}_c^{\mathrm{T}} \quad \mathbf{y}_e^{\mathrm{T}}\}$. In order to estimate $y_e(x^{(n_e+1)})$, we maximize the likelihood estimate function and get the following formula:

$$-\frac{1}{2}(\tilde{\mathbf{y}} - \mathbf{1}\mu)^{\mathrm{T}}\tilde{\mathbf{C}}^{-1}(\tilde{\mathbf{y}} - \mathbf{1}\mu) \tag{2.3}$$

or expressed as

$$-\frac{1}{2}\begin{pmatrix}\mathbf{y} - \mathbf{1}\hat{\mu} \\ \hat{y}_e(x^{(n_e+1)}) - \hat{\mu}\end{pmatrix}^{\mathrm{T}}\begin{pmatrix}\mathbf{C} & \mathbf{c} \\ \mathbf{c}^{\mathrm{T}} & \hat{\rho}^2\hat{\sigma}_c^2 + \hat{\sigma}_d^2\end{pmatrix}^{-1}\begin{pmatrix}\mathbf{y} - \mathbf{1}\hat{\mu} \\ \hat{y}_e(x^{(n_e+1)}) - \hat{\mu}\end{pmatrix},$$

where $\tilde{\mathbf{C}}$ is the correlation matrix given by