Variable-fidelity surrogate modelling with Kriging

Selvakumar Ulaganathan, Ivo Couckuyt, Francesco Ferranti, Tom Dhaene, Eric Laermans

Abstract—Variable-fidelity surrogate modelling offers an efficient way to approximate function data available in multiple degrees of accuracy each with varying computational cost. In this paper, a Kriging-based variable-fidelity surrogate modelling approach is introduced to approximate such deterministic data. Initially, individual Kriging surrogate models, which are enhanced with gradient data of different degrees of accuracy, are constructed. Then these Gradient enhanced Kriging surrogate models are strategically coupled using a recursive CoKriging formulation to provide an accurate surrogate model for the highest fidelity data. While, intuitively, gradient data is useful to enhance the accuracy of surrogate models, the primary motivation behind this work is to investigate if it is also worthwhile incorporating gradient data of varying degrees of accuracy.

Keywords—Kriging, CoKriging, Surrogate modelling, Variable-fidelity modelling, Gradients.

I. Introduction

The analysis and optimization of physics-based simulation codes require a significant investment of computational time and resources, despite a substantial advancement in computing power in the recent years. One of many ways of circumventing this problem is by constructing cheap approximations, known as surrogate models, for the expensive physics-based simulation codes. Surrogate modeling is successfully applied to model low dimensional problems with various techniques such as Artificial Neural Networks, Kriging, Support Vector Machines etc. A thorough description of various surrogate modeling techniques is given in [1], [2] and [3]. In this respect, various attempts to enhance the accuracy of surrogate models with secondary information such as gradients, Hessian data, cheap function data, etc. have been carried out in literature in recent years [4], [5], [6], [7], [8]. For example, additional gradient data is used to enhance the accuracy of Artificial Neural Networks based surrogate models in [9] and [10].

Kriging surrogate models are popular for approximating deterministic and computation-intensive simulation codes [11]. Direct incorporation of gradient data in Kriging was first introduced by Morris et al. in [5] and was further explored by various researchers in [6], [7], [12]. Incorporating gradients, either directly or indirectly, in Kriging is observed to significantly increase the accuracy of the surrogate models while requiring less training data [5], [6], [12]. Yamazaki et al. [4] incorporated first-order and second-order gradient data in Kriging and showed that gradient and Hessian data incorporation resulted in more accurate surrogate models than the models based on function data only. Liu incorporated gradient data in an integrated mean squared error-based Kriging formulation, but its performance is lower than that of incorporating gradients indirectly in Kriging [7].

Function data of varying degrees of accuracy can also be used to enhance the accuracy of the Kriging surrogate model. This approach is commonly known as CoKriging. Data (function+gradients) of different fidelities can be obtained in various areas of science and engineering with computational fluid dynamics (CFD) and finite element (FE) analysis being most popular due to their very expensive nature. Data of different fidelities can be either obtained by solving mathematically different simulation codes or by solving a single simulation code on meshes with different resolution or with different convergence criteria . For instance, gradient data of different fidelities can be cheaply obtained in FE/CFD applications with the use of perturbation analysis or adjoint and automatic differentiation tools. Function data of different fidelities are initially coupled in [13] with a linear regression formulation. An autoregressive formulation based multi-fidelity surrogate modelling is further introduced in [14] and is observed to be efficient in [15]. A multi-fidelity Kriging model enhanced with two different fidelities of gradient data in an optimization context is demonstrated in [16], but its advantage over the standard multi-fidelity Kriging model without gradients in finding global optima is still ambiguous.

In this work, the recently introduced recursive multi-fidelity Kriging formulation [17] is adapted to directly cope with different fidelities of function and gradient data to enhance the accuracy of the overall surrogate model. In this context, analytical expressions for the derivatives of the Matérn $\frac{5}{2}$ correlation function are derived and the recursive formulation based Gradient enhanced CoKriging (GCoK) approach is introduced in this work. The approach is demonstrated on an analytical problem and subsequently applied to solve a real-life problem. While gradient data is already proven to be useful in enhancing the accuracy of a surrogate model, this work extends the investigation on whether including gradient data of varying degrees of accuracy is also beneficial.

The reminder of the paper is organized as follows. The mathematical formulation of the GCoK approach is provided in Section II after a brief overview of Kriging. The formulation of the analytical and the simulation-based examples are given in Section III. Section III further discusses the results of the analytical and the simulation-based examples. Finally, Section IV summarizes the conclusions.

II. Mathematical Formulation

The standard Kriging prediction $\hat{y}(\boldsymbol{x}^*)$ at an untried prediction point $\boldsymbol{x}^*$ is expressed as a summation of a constant trend function $\hat{\mu}$ and a realization of a stationary Gaussian random

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process:

$$\hat{y}(\boldsymbol{x}^*) = \hat{\mu} + \boldsymbol{\psi}^T \boldsymbol{\Psi}^{-1}(\boldsymbol{y} - \boldsymbol{f}\hat{\mu}), \tag{1}$$

where $\boldsymbol{\psi}$ is a correlation vector which contains the correlation between the sample data and $\boldsymbol{x}^*$, $\boldsymbol{y}$ is a column vector of function values of the sample data, $\boldsymbol{f}$ is a column vector of ones, $\boldsymbol{\Psi}$ denotes the correlation matrix which contains the correlation between the sample data points and the constant trend function $\hat{\mu}$ is defined by generalized least squares,

$$\hat{\mu} = (\boldsymbol{f}^T \boldsymbol{\Psi}^{-1} \boldsymbol{f})^{-1} \boldsymbol{f}^T \boldsymbol{\Psi}^{-1} \boldsymbol{y}. \tag{2}$$

Here, in this work, the Matérn $\frac{5}{2}$ correlation function (see Appendix A) is used to calculate the correlation between the sample data.

The recursive formulation based CoKriging (CoK) estimate $\hat{y}^{CoK}(\boldsymbol{x}^*)$, which is considered as a multi-function extension to the standard Kriging estimate, can be expressed as,

$$\hat{y}^{CoK}(\mathbf{x}^*) = \rho \hat{y}_c(\mathbf{x}^*) + \hat{y}_d(\mathbf{x}^*), \tag{3}$$

where $\hat{y}_c(\mathbf{x}^*)$ is the function estimate from a standard Kriging model built with cheap data ($\mathbf{X}_c$, $\mathbf{y}_c$), $\hat{y}_d(\mathbf{x}^*)$ is the function estimate from a standard Kriging model built with residuals of the scaled cheap data and the expensive data ($\mathbf{X}_e$, $\mathbf{y}_d = \mathbf{y}_e - \rho\hat{\mathbf{y}}_c(\mathbf{X}_e)$) and ρ is the scaling parameter which is calculated along with the hyper-parameters ($\theta_m, m = 1, ..., k$, where k is the dimensionality of the function) of the Matérn $\frac{5}{2}$ correlation function using a maximum likelihood estimation method. The recursive formulation based CoKriging results in equivalent prediction as standard CoKriging when the expensive data is a subset of the cheap data.

In this work, additional gradient data of two degrees of accuracy (i.e., cheap and expensive gradient data) are incorporated in the recursive formulation of CoKriging and thus Equation 3 becomes,

$$\hat{y}^{GCoK}(\mathbf{x}^*) = \rho \hat{y}_c^{GEK}(\mathbf{x}^*) + \hat{y}_d^{GEK}(\mathbf{x}^*), \tag{4}$$

where $\hat{y}_c^{GEK}(\mathbf{x}^*)$ is the function estimate from a Gradient Enhanced Kriging (GEK) model built with cheap data ($\mathbf{X}_c$, $\dot{\mathbf{y}}_c$) and $\hat{y}_d^{GEK}(\mathbf{x}^*)$ is the function estimate from a GEK model built with residuals of the scaled cheap data and the expensive data ($\mathbf{X}_e$, $\dot{\mathbf{y}}_d = \dot{\mathbf{y}}_e - (\hat{\mathbf{y}}_c^{GEK(\mathbf{X}_e)}, \frac{\partial}{\partial \mathbf{x}}(\hat{\mathbf{y}}_c^{GEK(\mathbf{X}_e)})^T)$. The notation $\dot{\mathbf{y}}$ represents that the vector $\mathbf{y}$ now contains both the function and the gradient data. A GEK estimate $\hat{y}^{GEK}(\boldsymbol{x}^*)$ at the untried prediction point $\boldsymbol{x}^*$ is expressed as,

$$\hat{y}^{GEK}(\boldsymbol{x}^*) = \hat{\dot{\mu}} + \dot{\boldsymbol{\psi}}^T \dot{\boldsymbol{\Psi}}^{-1}(\dot{\boldsymbol{y}} - \boldsymbol{f}\hat{\dot{\mu}}), \tag{5}$$

where

$$\dot{\boldsymbol{\Psi}} = \begin{Bmatrix} \boldsymbol{\Psi} & \frac{\partial \boldsymbol{\Psi}}{\partial x_1^{(i)}} & \cdots & \frac{\partial \boldsymbol{\Psi}}{\partial x_v^{(i)}} & \cdots & \frac{\partial \boldsymbol{\Psi}}{\partial x_k^{(i)}} \\ \frac{\partial \boldsymbol{\Psi}}{\partial x_1^{(j)}} & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_1^{(i)} \partial x_1^{(j)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_1^{(i)} \partial x_v^{(j)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_1^{(i)} \partial x_k^{(j)}} \\ \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\ \frac{\partial \boldsymbol{\Psi}}{\partial x_u^{(j)}} & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_1^{(j)} \partial x_u^{(i)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_u^{(i)} \partial x_v^{(j)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_u^{(i)} \partial x_k^{(j)}} \\ \vdots & \vdots & \cdots & \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{\Psi}}{\partial x_k^{(j)}} & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_1^{(j)} \partial x_k^{(i)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_v^{(j)} \partial x_k^{(i)}} & \cdots & \frac{\partial^2 \boldsymbol{\Psi}}{\partial x_k^{(i)} \partial x_k^{(j)}} \end{Bmatrix}, \tag{6}$$

$$\dot{\boldsymbol{\psi}} = \left(\boldsymbol{\psi}, \frac{\partial \boldsymbol{\psi}}{\partial x_1}, ..., \frac{\partial \boldsymbol{\psi}}{\partial x_k} \right)^T, \tag{7}$$

$$\dot{\boldsymbol{y}} = \left(\boldsymbol{y}, \frac{\partial \boldsymbol{y}}{\partial x_1}, ..., \frac{\partial \boldsymbol{y}}{\partial x_k} \right)^T, \tag{8}$$

$$\boldsymbol{f} = \left(1_1, ...1_n, 0_{n+1}, ..., 0_{(k+1)n} \right)^T, \tag{9}$$

where n is the number of training sample points, $\dot{\boldsymbol{\Psi}}$ is a $(k+1)n \times (k+1)n$ symmetric block matrix and contains the correlations of function and gradient data between the sample data points and the correlation vector $\dot{\boldsymbol{\psi}}$ contains the correlation of both function values and gradients between the sample data and $\boldsymbol{x}^*$. The vector $\dot{\boldsymbol{y}}$ contains both the function values and the gradients of the sample data. The notations $\partial \boldsymbol{\Psi} / \partial x_u^{(j)}$ and $\partial^2 \boldsymbol{\Psi} / \partial x_u^{(i)} \partial x_v^{(j)}$ denote the correlation between function data and u^{th} dimension gradients and correlation between u^{th} dimension gradients and v^{th} dimension gradients, respectively. The direction of differentiation is denoted by i and j with $x^{(i)}$ and $x^{(j)}$ denoting two different samples.

III. Results and Discussion

A. Problem Formulation

Gradient enhanced CoKriging is applied to two benchmark problems and compared against standard CoKriging. Normalized Root Mean Square Error (NRMSE) on a validation data set of n_p pseudorandom points is used to assess the accuracy of the surrogate models and can be expressed as,

$$NRMSE = \frac{\sqrt{\frac{\sum_{i=1}^{n_p} \left(y_t^i - \hat{y}^{GCoK^i} \right)^2}{n_p}}}{max(\boldsymbol{y}_t) - min(\boldsymbol{y}_t)}, \tag{10}$$

where $\hat{\boldsymbol{y}}^{CoK}$ contains the estimated response values and $\boldsymbol{y}_t$ denotes the true response values.

B. Analytical Problem

Expensive and cheap versions of the analytical function are defined as,

$$f_e(x) = (6x - 2.0)^2 sin(12x - 4.0), x \in [0, 1] \tag{11}$$

and

$$f_c(x) = 0.5(f_e(x)) + 10(x - 0.5) - 5, \tag{12}$$

respectively. The design space is equidistantly sampled at 2 expensive and 7 cheap sample points. Intuitively, both CoKriging and GCoK interpolate the expensive data and use the cheap data to approximate the trend of the actual function. The CoKriging approximation with just 2 expensive sample points gives a poor prediction whereas the gradient incorporation at both the expensive and the cheap sample points allows the GCoK model to not only accurately capture the actual function trend but also to accurately overlay the actual function behaviour (see Figure 1). This observation is further supported by the results shown in Table I.

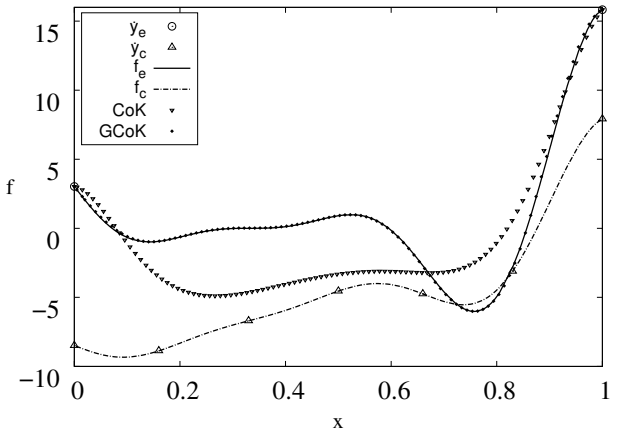


Fig. 1: CoKriging with $n_e = 2$ and $n_c = 7$ and GCoK with $n_e = 2$ + gradients and $n_c = 7$ + gradients. (1D Function)

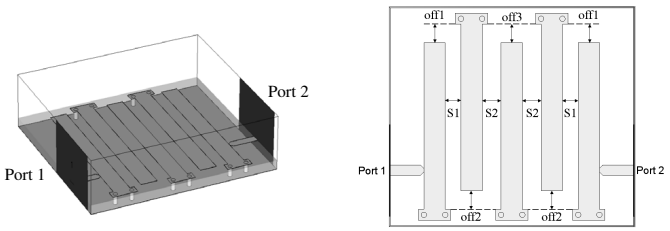
TABLE I: NRMSE on a validation data set of $n_p = 500$ with $n_e = 2$ and $n_c = 7$. Imp. denotes "% of improvement" of GCoK model over its corresponding CoKriging model. (1D analytical function)

Model	NRMSE	Imp.
CoK	0.1459	-
GCoK	0.0049	96%

C. Real-life problem

The real-life example involves modelling of the mean of magnitude of the scattering S_{11} parameter of a microwave inter-digital filter, denoted by $|S_{11}|_{mean}$, in the frequency range $[2.2 - 2.6]$ GHz with the ulterior goal of optimization (though not the focus of this paper). The inter-digital filter is parameterised using 5 geometrical parameters (see Figure 2). The function and gradient data of two different fidelities are obtained by carrying out full-wave electromagnetic simulations on two meshes of varying refinement (a coarse mesh with 7823 tetrahedral cells and a dense mesh with 48000 tetrahedral cells) using CST MicroWave Studio[2]. The computation time of converging to a solution on the dense mesh (i.e., high-fidelity data) is about $900s$ whereas it is about $130s$ on the coarse mesh (i.e., low-fidelity data). The computation time of acquiring one function value is roughly equal to that of acquiring 10 and 20 sets of 5-dimensional gradients for the dense and coarse meshes, respectively. Adding gradient data results in a significant accuracy improvement in GCoK models over the CoKriging models (see Table II and Figure 3). GCoK models essentially benefit from the fact that the Kriging interpolation is now constrained by both function and gradient data which allows them to successfully capture the actual covariance structure with less number of sample points. More accurate GCoK models than CoKriging models are obtained even when only introducing gradient data at X_e (see Figure 4). However, incorporating gradient data only at X_c, in general, does not provide much advantage to GCoK models (see Figure 5).

[2]CST Computer Simulation Technology AG, Darmstadt, Germany, *www.cst.com*



(a) CST Model

(b) Top view

Fig. 2: The 5 geometric parameters implicitly define the length of the microstrips ($off1$, $off2$ and $off3$) and the spacing between the microstrips ($S1$ and $S2$).

TABLE II: NRMSE on a validation data set of $n_p = 50$ with $n_e = 50$ and $n_c = 100$. Imp. denotes "% of improvement" of GCoK model over its corresponding CoKriging model. ($|S_{11}|_{mean}$ 5D)

Model	NRMSE	Imp.
CoK	0.0524	-
GCoK	0.0297	43%

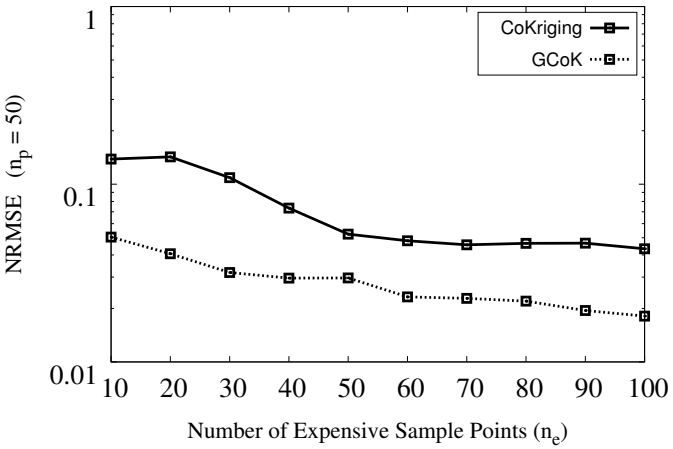


Fig. 3: Evolution of NRMSE on a validation data set of $n_p = 50$ for a varying number of expensive data. A constant number of cheap data $n_c = 100$ is used for the expensive runs. ($|S_{11}|_{mean}$ 5D)

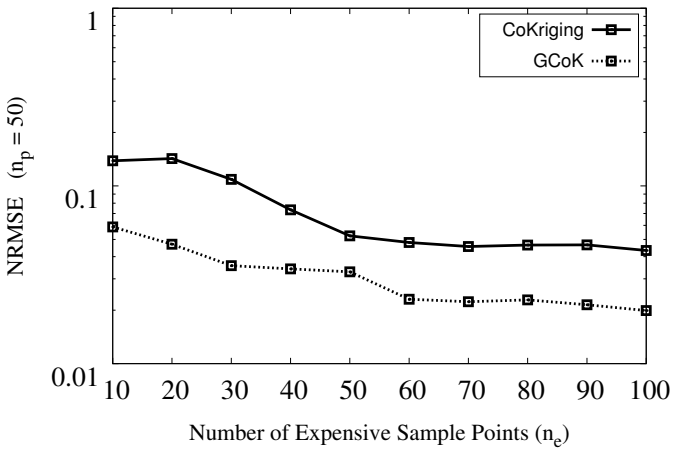


Fig. 4: Evolution of NRMSE on a validation data set of $n_p = 50$ for a varying number of expensive data. A constant number of cheap data $n_c = 100$ is used for the expensive runs, but no gradient data is incorporated at X_c. ($|S_{11}|_{mean}$ 5D)

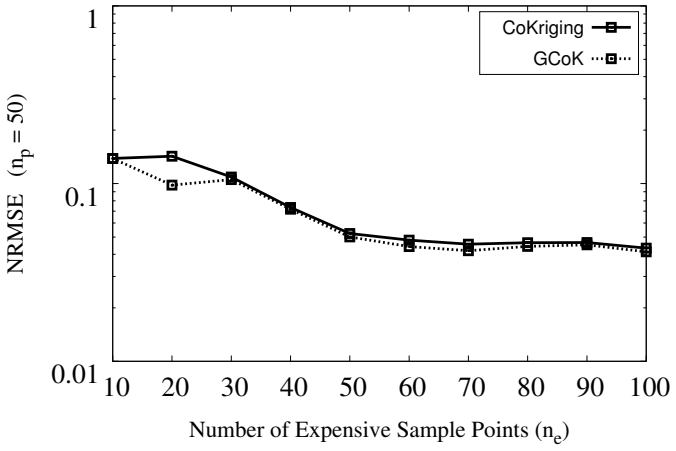


Fig. 5: Evolution of NRMSE on a validation data set of $n_p = 50$ for a varying number of expensive data. A constant number of cheap data $n_c = 100$ is used for the expensive runs, but no gradient data is incorporated at X_e. ($|S_{11}|_{mean}$ 5D)

IV. Conclusion

A Kriging-based variable-fidelity surrogate modelling approach is introduced. Test results show that incorporating additional gradient data of varying degrees of accuracy can significantly enhance the accuracy of the Kriging-based variable-fidelity surrogate model. Moreover, incorporating only the highest fidelity gradient data itself results in more accurate surrogate models than CoKriging models without gradient data. However, when the accuracy of the gradient data becomes too worse, the advantage which can be reaped from the gradient data of fidelities other than the highest fidelity becomes negligible.

Appendix A

Matérn $\frac{5}{2}$ correlation function:

$$\psi_{\nu=\frac{5}{2}}(d) = (1 + \sqrt{5}a + \frac{5a^2}{3})exp\left(-\sqrt{5}a\right), \qquad (13)$$

where $d = |x_m^i - x_m^j|$ and $a = \sqrt{\sum_{m=1}^{k} \theta_m d_m^2}$.

Gradient of correlation function with respect to X (i.e., cross-correlation):

$$\frac{\partial \mathbf{\Psi}^{(i,j)}}{\partial x^{(j)}} = \frac{5\theta d(\sqrt{5}a + 1)exp\left(-\sqrt{5}a\right)}{3} \qquad (14)$$

Hessian of correlation function with respect to X (i.e., cross-correlation):

$$\frac{\partial^2 \mathbf{\Psi}^{(i,j)}}{\partial x_u^{(i)} \partial x_v^{(j)}} = \begin{cases} \frac{-25\theta_u \theta_v d_u d_v exp\left(-\sqrt{5}a\right)}{3} & \text{if } u \neq v \\ \left[\frac{-25\theta^2 d^2 + 5\theta(\sqrt{5}a+1)}{3}\right] exp\left(-\sqrt{5}a\right) & \text{if } u = v \end{cases} \qquad (15)$$

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