Surrogate modeling of two nested codes with a functional intermediary variable

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Abstract:

A lot of industrial problems involve multi-physics phenomena, which can be associated with a network of nested computer codes. If this code network is used for conception, uncertainty quantification, or risk analysis purposes, its output has to be evaluated in a huge number of points. If the associated computer codes are computationally expensive, surrogate models have to be introduced to predict the quantity of interest.

In this work, our aim is to predict the output of a chain of two codes, with a small computational budget. Each code has a functional output. The functional output of the first code is an input of the second code. The associated formalism can thus be written:

$$\begin{array}{ccccc} & & \boldsymbol{x}_2 & & \\ & & & \searrow & \\ \boldsymbol{x}_1 & \rightarrow & \boldsymbol{y}_1(\boldsymbol{x}_1) & \nearrow & \boldsymbol{y}_2(\boldsymbol{y}_1(\boldsymbol{x}_1), \boldsymbol{x}_2), \end{array} \tag{1}$$

where $\boldsymbol{x}_1$, and $\boldsymbol{x}_2$ are the vectors of scalar inputs of the two codes and $\boldsymbol{y}_1$ et $\boldsymbol{y}_2$ the discretized functional outputs of the codes, $\boldsymbol{y}_1(\boldsymbol{x}_1) := (y_1(\boldsymbol{x}_1, t_1), \ldots, y_1(\boldsymbol{x}_1, t_{N_t}))$ and $\boldsymbol{y}_2(\boldsymbol{y}_1(\boldsymbol{x}_1), \boldsymbol{x}_2) := (y_2(\boldsymbol{y}_1(\boldsymbol{x}_1), \boldsymbol{x}_2, t_1), \ldots, y_2(\boldsymbol{y}_1(\boldsymbol{x}_1), \boldsymbol{x}_2, t_{N_t}))$.

To build surrogate models, we use Gaussian process modeling. In this framework, the output of an expensive code can be *a priori* modeled by a Gaussian process. Then a Gaussian predictor of the output of the code is obtained by computing the *a posteriori* distribution of the process given observations of the code. The Gaussian process modeling is widely used [3, 4] for codes with scalar or low dimensional inputs and outputs. Moreover, a code network is generally regarded as a single code, and the observations of the intermediary variables are not taken into account.

In our case, several distinctive features appear. The first code has scalar inputs and a functional output and the second one has scalar and functional inputs and a functional output. Finally, the quantity of interest is the functional output of the chain of codes.

We propose first a method to predict this quantity of interest for a given set of observations of the two codes. An interesting property of the predictor obtained, is that it can take into account observations of the intermediary variable, or of one of the codes only. The predictor is obtained by treating the specific features as follows.

First, the dimension of the functional input of the second code is reduced. This enables to reduce the surrogate modeling of the second code to the surrogate modeling of a code with

scalar inputs and a functional output. Two dimension reduction techniques are proposed : the first one is based on a Principal Component Analysis of the functional input, the second one is output-oriented and is based on the assumption that the output can be approximated by the form $A\boldsymbol{y_1}(\boldsymbol{x_1})$, with A a $N_t \times N_t$-dimensional matrix.

The surrogate models of both codes have now only scalar inputs and a functional output. The surrogate modeling of a code with scalar inputs and a functional output is made thanks to a Gaussian process with a tensorized covariance function.

Once a Gaussian predictor of each code is obtained, the predictors can be coupled to obtain a predictor of the output of the nested code. However, the coupling of two Gaussian processes is not Gaussian. We therefore propose a linearization of this coupling of the predictors to obtain a Gaussian predictor of the nested code.

Thus, thanks to a dimension reduction of the functional input of the second code, a tensorized structure of the covariance function and a linearization of the coupling of the predictors of the codes, a Gaussian predictor of the nested code can be obtained. This predictor is built with the Gaussian processes conditioned by observations of the two codes.

Second, we propose sequential design methods in order to improve the nested code prediction accuracy. Existing methods generally deal with a scalar or low-dimensional quantity of interest and the criteria for adding a new observation point are based on a reduction of the prediction variance of this quantity [3, 4, 1]. We propose two methods based on a reduction of the prediction variance [2]. Thanks to the tensorized covariance functions, the criteria of the methods can be evaluated fast. Indeed, this tensorized structure implies to inverse a huge number of times $N_{x_i} \times N_{x_i}$-dimensional matrices , $i \in \{1, 2\}$, instead of $N_t N_{x_i} \times N_t N_{x_i}$ for a non-tensorized structure, where N_{x_1} and N_{x_2} are the number of observations of the codes.

The first sequential design method corresponds to the case of an indivisible chain of codes. The second one corresponds to the case when the computer codes can be launched separately. This second method takes advantage of the nested structure of the codes in order to improve the prediction accuracy at a given computational budget. It enables also to take into account different computational costs of the two codes.

References

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Short biography – Graduate from Ecole Centrale de Lyon in 2010, I have worked for 4 years as engineer in building energy performance. In 2014-2015 I have studied in M2 ISIFAR at Université Paris Diderot Paris 7 and I have done an internship in applied mathematics at CEA. Then I have pursued with a PhD in "Surrogate modelling of complex systems", which began in November 2015.