

Towards Optimization of Multi-Material Structure: Metamodeling of Mixed-Variable Problems

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ABSTRACT

In structural design optimization, it is challenging to determine the optimal dimensions and material for each component simultaneously. Material selection of each part is always formulated as a categorical design variable in structural optimization problems. However, it is difficult to solve such mixed-variable problems using the metamodelbased strategy, because the prediction accuracy of metamodels deteriorates significantly when categorical variables exist. This paper investigates two different strategies of mixed-variable metamodeling: the “feature separating” strategy and the “all-in-one” strategy. A supervised learning-enhanced cokriging method is proposed, which fuses multi-fidelity information to predict new designs’ responses. The proposed method is compared with several existing mixed-variable metamodeling methods to understand their pros and cons. These methods include Neural Network (NN) regression, Classification and Regression Tree (CART) and Gaussian Process (GP). This study provides insights and guidance on the establishment of proper metamodels for multi-material structural design problems.

Keywords: Multi-material, Mixed-variable, Cokriging, Neural Network, Classification and regression tree, Gaussian, Supervised learning

CITATION: Xu, H., Chuang, C., and Yang, R., "Towards Optimization of Multi-material Structure: Metamodeling of Mixed-Variable Problems," *SAE Int. J. Mater. Manf.* 9(2):2016, doi:10.4271/2016-01-0302.

1. INTRODUCTION

To further improve vehicle fuel efficiency and reduce emissions, lightweighting techniques have attracted great attention in recent years. One technique for lightweight vehicle components is to replace traditional materials with various types of advanced materials, such as high-strength steel, aluminum and carbon fiber composites. Therefore, multi-material structure is considered as the future trend of lightweighting [1, 2, 3, 4].

To design a multi-material structure, the most proper material will be selected for each part to achieve the optimal system-level performances. Parametric optimization of multi-material structure involves both continuous design variables (e.g. dimension of components), discrete variables (e.g. the number of drilled holes), and categorical variables (e.g. selection from the candidate materials). The categorical variables are used to represent any nonnumerical data, which can be either ordered (ordinal variables) or non-ordered (nominal variables). A general formulation of the mixed-variable design optimization is shown as follows:

Minimize:

$$y = f(\mathbf{x}, \mathbf{c}) \quad (1)$$

Subject to:

$$g(\mathbf{x}, \mathbf{c}) < 0 \quad (2)$$

$$h(\mathbf{x}, \mathbf{c}) = 0 \quad (3)$$

where $\mathbf{x}$ is a vector of the continuous design variables; $\mathbf{c}$ is a vector of the discrete and categorical variables; y is the design objective; g and h are the design constraints.

In engineering design problems, advanced computer models are widely employed to evaluate the objective function $f(\mathbf{x}, \mathbf{c})$ and the constraint functions $g(\mathbf{x}, \mathbf{c})$, $h(\mathbf{x}, \mathbf{c})$. The advanced simulations are time consuming and computationally expensive. As a cheap replacement of the expensive simulations, metamodels (surrogate models) are established on a set of sample points generated by Design of Experiments (DOE). The metamodel-based design optimization method has been widely accepted as an efficient tool of computational engineering design. T. Simpson [5] and R. Jin [6] have conducted surveys and comparative studies on existing continuous variable metamodeling methods. Recommendations are made for different types of design problems. Polynomial regression, Neural Networks (NN) [7, 8], Kriging [9, 10, 11], Multivariate Adaptive Regression Splines (MARS) [12] and Radial Basis Function (RBF) [13, 14] are reviewed in these works.

However, the majority of the existing metamodels are developed for continuous input variables. The categorical inputs are ordered in some way and coded numerically when the continuous-variable metamodels are applied on the mixed-variable problems. In some cases, such treatment can lead to undesirable and misleading results [15, 16]. There are fewer metamodeling techniques that can handle the categorical variables. To extend the metamodeling methods to mixed variable problems, two main strategies can be followed:

- “All-in-one” strategy. A single unified model is established to handle all design variables. For example, the categorical variables are coded as numerical variables in Gaussian Process (GP) modeling or Treed Gaussian Process (TGP) modeling [17, 18]. Another well-known method is NN [7, 8, 19]. An NN is composed of neurons which are multiple linear regression models with a nonlinear transformation on the output. The process of training a NN model is to assemble the neurons following a certain structure, and to predict the associated weights based on the training data. A recent study [20] reports that NN generates better predictions than the nonlinear regression models.
- “Feature separating” strategy. Separate kernels/surrogate models are established respectively to describe different “features” that are observed from training data. Multiple Kernel Regression (MKR) models [20, 21] are developed following this philosophy. Classification and Regression Tree (CART) [22, 23] also belongs to this category, which can predict the value of continuous responses from a set of continuous and categorical predictor variables.

Multi-material structural design is distinguished from other mixed-variable problems by one important feature: structural responses have similar or even very close trends when different materials are selected. In certain special cases such as linear elastic analysis, the material candidates can be perfectly coded by numerical values without introducing errors. For example, only elastic modulus is involved in elastic deformation analysis and Noise Vibration and Harshness (NVH) analysis, etc. Therefore, the candidate materials can be sorted and coded by their elastic modulus. On the other hand, when large deformation and failure occurs, it is impossible to find a simple linear relation between the material code and the structural behavior. However, different but similar trends in structural behaviors can still be observed, if two materials (MAT I and MAT II) have similar constitutive relations. Structural behavior of MAT II can be considered as “low fidelity” information to supplement the prediction of structural behaviors of MAT I. The purpose of this paper is to better understand the relative merits of mixed-variable metamodeling methods in multi-material structure design problems. Comparative studies are conducted using two engineering benchmark problems. We also propose a new supervised learning-based method to process and prepare the training data for “feature separating” metamodeling strategies such as cokriging. The remainder of this paper is organized as follows: in Section 2, a new supervised learning-aided cokriging metamodeling method is introduced. In Section 3, a brief review of

several other metamodeling methods is also provided. In Section 4, two comparative studies are conducted on those metamodeling methods. Section 5 is the summary.

2. A SUPERVISED LEARNING-AIDED FEATURE SEPARATING METAMODELING STRATEGY

2.1. Review of Cokriging Method

In cokriging, the prediction of a design point’s response, on the basis of the neighbor values of one or several other training point, is the best possible according to the following two statistical criteria:

- Minimization of the error between the true responses and the predicted responses on the training points;
- Minimization of the variance of the estimations.

Compared to the ordinary kriging, cokriging has some unique features. For a design problem of multiple responses, cokriging can effectively utilize the information of a secondary response, which is cross-correlated with the primary response of interest. If the secondary response is easier and cheaper to obtain (e.g. more DOE samples are available), the responses of unknown points can be predicted using both the data within individual specified grade categories, as well as the neighboring values of other categories.

Consideration of the cross-correlation improves the accuracy of predicting new designs’ responses. When it is applied to multimaterial problems, cokriging is able to capture (1) structural behaviors induced by each material, and (2) the similarity/correlation in structural behaviors of different materials.

According to references [24, 25, 26], the cokriging metamodel is formulated as a linear combination of both primary and secondary data values:

$$z_0^* = \sum_{i=1}^n \alpha_i z_i + \sum_{j=1}^m \beta_j t_j \quad (4)$$

where z_0^* is the prediction of a new design’s response at location $\mathbf{x}_0$ in the design space; α_i is the weight assigned to the samples of the primary response z_i ; β_j is the weight assigned to the samples of the secondary response t_j ; z_i and t_j are functions of design variables $\mathbf{x} = \mathbf{x}_0$. n nearby locations to the design $\mathbf{x}_0$ are sampled for the primary response, and m nearby locations to the design $\mathbf{x}_0$ are sampled for the secondary response.

The development of the co-kriging metamodel is the same as the development of the ordinary kriging system. The prediction error of a cokriging model is expressed as:

$$E = \sum_{i=1}^n \alpha_i z_i + \sum_{j=1}^m \beta_j t_j - z_0 \quad (5)$$

where z_0 is the true response of the design $\mathbf{x}_0$. The variance of prediction error in terms of the cokriging weights and the covariance between the responses is expressed as:

$$\begin{aligned} Var(E) = & \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j cov\{z_i z_j\} + \sum_{i=1}^m \sum_{j=1}^m \beta_i \beta_j cov\{t_i t_j\} + 2 \\ & \cdot \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j cov\{z_i t_j\} - 2 \cdot \sum_{i=1}^n \alpha_i cov\{z_i z_0\} - 2 \\ & \cdot \sum_{j=1}^m \beta_j cov\{t_j z_0\} + cov\{z_0 z_0\} \end{aligned} \quad (6)$$

For the simplest case of 1 material selection variable and 2 candidate materials, the cokriging method can be directly applied. The material of interest is selected as primary, and the other material is selected as secondary.

2.2. Cokriging of the Simplest Mixed-Variable Case: 1 Material Selection Variable, 2 Candidate Materials

In this work, it is assumed that the choices of different materials lead to not the same but similar trends of structural behaviors (Figure 1). The design variables consist of two parts: the structure dimension variables $\mathbf{x}$, and the material selection variables $\mathbf{c}$. The primary response is marked as $\mathbf{z}$, and the other responses are marked as $\mathbf{t}$. The following notations are used throughout this paper:

- The $\mathbf{x} - \mathbf{z}$ and $\mathbf{x} - \mathbf{t}$ relations of a given $\mathbf{c}$ is referred as the “response functions”.
- $\mathbf{x} - \mathbf{z}$ relation is the “primary” response function;
- The $\mathbf{x} - \mathbf{t}$ relation is the “secondary” response function.

To predict the structural behaviors of MAT 1, the DOE points of MAT 1 are selected as the primary training data; the DOE points of MAT 2 are selected as the secondary training data. A cokriging metamodel is established on the primary and secondary dataset to predict the behaviors of a new structure design of MAT 1.

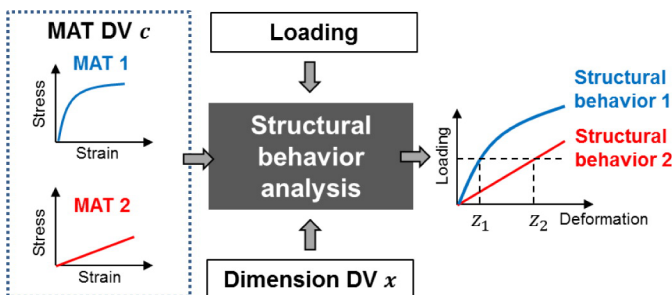


Figure 1. An illustrative example of material property-structural behavior relation. “DV” stands for “Design Variables”

2.3. Cokriging of the Multiple Mixed-Variable Case: a Supervised Learning-Based Strategy

When there are more than 2 material selection design variables and multiple candidate materials, it is impractical to directly employ the “feature separating” strategy. For example, 3 material selection variable and 4 candidate materials will generate 64 combinations. If the training data is split into 64 subsets, there will be insufficient data for metamodel training of each material combination.

To resolve this issue, a supervised learning-aided method is proposed. The most important material selection variable is identified using the feature selection algorithm. All the other non-important material selection variables are coded numerically. The primary and secondary training datasets are determined for each response function. The flowchart of the proposed method is shown in Figure 2.

First, the training data is collected by DOE. The input factors of DOE are all the design variables, including both the continuous/discrete structural variables and the categorical material selection variables. The DOE points can be generated using any space filling method. It is recommended to use Latin Hypercube Sampling (LHS) or Optimized Latin Hypercube Sampling (OLHS) [27] if there is no prior knowledge about the preferable design region. This study doesn’t adopt any adaptive DOE methods due to their complexity. “One-shot DOE”, a.k.a. generating all DOE points in one step using space filling technique, is widely accepted as the common practice in industry because it can fully utilize the parallel computing technology. The proposed method aims to improve the accuracy of metamodeling without changing the existing DOE process, or requiring additional experiments.

Second, the key material selection variable is identified. A supervised learning feature selection algorithm, Relief [28, 29, 30], is employed for this purpose. The material selection variables are taken as input features, and the structural behaviors are taken as the supervisory signal. The key idea of the Relief algorithm is to estimate the quality of attributes (input features) according to how well their values distinguish between instances (training samples) that are near to each other within a local context. Taking DOE points as the training data, the Relief algorithm will generate a ranking and weights of all input variables. The material selection variable of the largest weight is identified as the key variable (c_k). The dataset is separated into M subsets according to c_k ’s value (M candidate materials). For other non-important material selection variables, the candidate materials are ordered by their strength and coded numerically (e.g. 0, 1, 2, 3, ...).

Third, the primary training dataset is determined. To metamodeling the response function of $c_k = i$, subset i is chosen as the primary dataset.

Forth, the secondary dataset is determined. For $c_k = 1, 2, \dots, M$ and $c_k \neq i$, a kriging model is established for each material selection. The accuracy of the $M - 1$ metamodels are validated using subset i . A high accuracy indicates that the current subset has a high similarity to the primary dataset (subset i). The subset of the highest similarity is chosen as the secondary dataset.