Kriging with mixed kernel (MK) for complex aerospace problems

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ABSTRACT

Most complex aerospace problems are characterized as non-linear, non-smooth, noisy, and with heterogenous function profiles. In this paper, we propose a novel kriging variant to address its current limitations to approximate such problems. In particular, we explore the mixed kernel (MK) approach, which enables selecting a different kernel function for each variable. This approach provides a means to better model the inherent heterogeneity of the complex function. For benchmarking purpose, we use two analytical and one engineering case studies. The performance is compared to those obtained from using a single kernel, ensemble method and the composite kernel learning (CKL). Overall, the MK approach is shown to be superior in terms of computational accuracy, though it incurs additional computational cost, especially for higher-dimensional problems.

1. Introduction

The complexity of aerospace systems and operations has increased immensely, driven by the continuous need for improvement in the industry. System complexity and stringent regulations drive the development process, where many factors and constraints need to be balanced to find a better solution [1]. Merging the different disciplines also represents an issue as it raises the number of constraints and inputs involved. Modeling an aircraft performance, for instance, requires the simultaneous considerations of aerodynamic, structures, propulsion, flight trajectory, atmospheric conditions, etc. Moreover, a design process typically involves performing optimization and uncertainty analysis, which require a large number of function evaluations. Such analyses will be computationally intractable to perform on a highly complex, multidisciplinary problem. Surrogate models have been commonly employed as cheaper representations of the original functions. It is thus imperative to ensure the approximation accuracy of the surrogate models, in order to have valid analysis results. The kriging surrogate model has been demonstrated successfully in various applications, including those in the context of aerospace engineering applications. The complexity of the physical system that needs to be modeled, however, could quickly surpass the modeling capability of the conventional kriging models. In this work, we aim to explore and develop kriging variants that offer more flexibility and thus are more suitable for the complex problems at hand. In particular, we introduce the flexibility in the kernel selection for each design variable in the kriging construction. Benchmarking is performed with analytical and aerodynamic test cases, and the computational accuracy and efficiency are discussed.

2. Method

Kriging approximates the relationship between the N_D-dimensional input, $\mathbf{x} = \left\{x^{(k)}\right\}_{k=1,\ldots,N_d}$, and the output, y of a blackbox function:

$$Y(\mathbf{x}) = \mu + Z(\mathbf{x}) \tag{1}$$

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where μ is the global model and $Z(\mathbf{x})$ is the stochastic component with a zero mean and covariance $\mathrm{Cov}[Z(\mathbf{x}), Z(\mathbf{x}')] = \sigma^2 \mathbf{R}(\mathbf{x}, \mathbf{x}')$. σ^2 is the variance and $\mathbf{R}(\cdot,\cdot)$ is the correlation matrix. The global model is assumed constant here, as we only consider the *ordinary kriging* model for this work. The selection of kernel for the correlation matrix is critical for kriging construction, as it encodes assumptions about the dependence structure of the function of interests. For higher-dimensional problems, the product correlation rule is typically used to construct the correlation matrix, where the correlation function can be expressed as a product of stationary, one-dimensional correlations. The correlation between the i-th and j-th samples can then be expressed as:

$$R_{ij}(\boldsymbol{\theta}, d) = \prod_{k=1}^{N_d} R\left(\theta^{(k)}, d_{ij}^{(k)}\right). \tag{2}$$

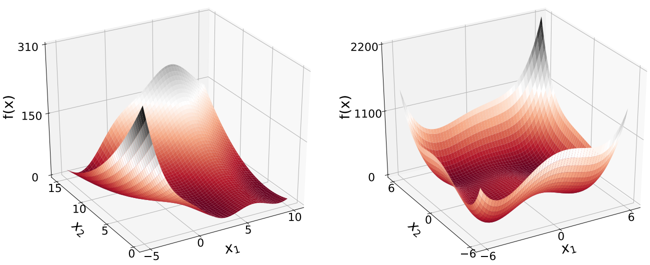
The vector of correlation parameters is denoted as $\boldsymbol{\theta} = \left\{\theta^{(k)}\right\}$, $k = 1, \ldots N_d$. The value $d_{ij}^{(k)}$ is the distance between two points in the k^{th} dimension, $\left|x_i^{(k)} - x_j^{(k)}\right|$.

Here we propose a novel mixed kernel (MK) approach, where each of the $R\left(\theta^{(k)}, d_{ij}^{(k)}\right)$ terms in Equation 2 can have a different kernel function. Each variable is treated as a separate entity, to better reflect the heterogeneity of real-world complex problems. At this stage, we consider all possible combinations of kernels before the best combination is selected. While this works well for the low-dimensional problems considered in this study, further investigation is required to efficiently search for the optimum kernel combination.

In this paper, for the single-kernel cases, we consider the Gaussian (G), Exponential (E), Matérn 3/2 (M3/2) and Matérn 5/2 (M5/2) kernels. The recently developed ensemble method (EM) and composite kernel learning (CKL) [2] are also considered. The ensemble method uses weights obtained from the Akaike Information Criterion (AIC) to combine the response surfaces from the four kernels. The CKL method constructs new covariance functions through the weighted combination of the four kernels.

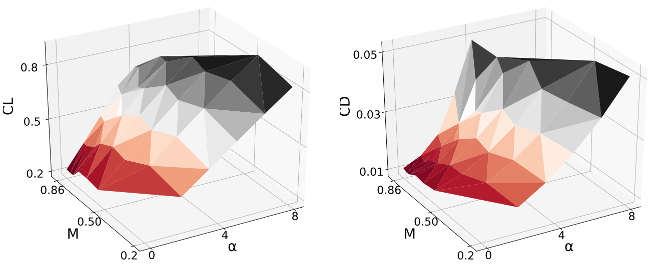
3. Test problems

The benchmarking test cases considered here include two analytical problems (Branin and Himmelblau functions) and an aerodynamic test case; all are two-dimensional problems. The Branin function is modeled with $x_1 \in [-5, 10]$ and $x_2 \in [0, 15]$, and the Himmelblau function is modeled with $x_1, x_2 \in [-6, 6]$; they are illustrated in Figure 1. The aerodynamic test case comprises the approximations of lift and drag coefficients (C_L and C_D) of a Common Research Model (CRM) configuration. To generate the samples, we run 3-D Reynolds-Averaged Navier Stokes (RANS) simulations on the SU2 solver[1], by varying the Mach number ($M \in [0.20, 0.86]$) and angle of attack ($\alpha \in [0.0°, 8.0°]$). The C_L and C_D profiles are shown in Figure 2.



(a) Branin function (b) Himmelblau function

Fig. 1: Function profiles of the analytical functions.



(a) Lift coefficient (b) Drag coefficient

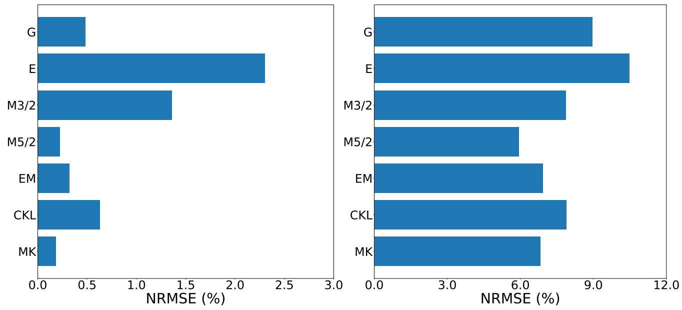
Fig. 2: Function profiles for the CRM problem.

4. Results and Discussion

We validate the surrogate models by computing the normalized root-mean square errors (NRMSE). Both Branin and Himmelblau functions are built with 20 Halton samples, and validated with 100 points. The CRM C_L and C_D approximations are tested with 100 independent runs to avoid biases in the results, each with 20 samples. The derived MK approach is compared against four single kernels, CKL, and the ensemble approach. The errors for the analytical test cases are shown in Figure 3, whereas the error bars (from the 100 runs) for the CRM problem are shown in Figure 4.

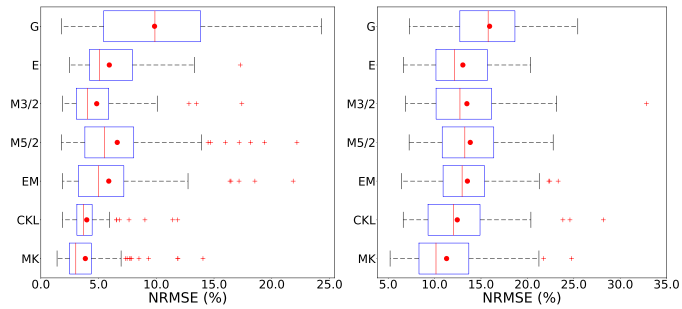
The single kernel performance is problem-dependent. We can observe from Figure 3 that the best single kernel is Matérn 5/2. Matérn 3/2 is shown to be the best for the C_L prediction (Figure 4a), whereas

[1] https://su2code.github.io/



(a) Branin function NRMSE. (b) Himmelblau function NRMSE.

Fig. 3: Approximation errors for the analytical tests.



(a) C_L NRMSE (b) C_D NRMSE

Fig. 4: Approximation errors for the CRM problem.

Gaussian is shown to be the worst for the C_D prediction (Figure 4b). Performance improvements are observed when we consider multiple kernels, led by the MK approach and followed by CKL. For the Himmelblau function, however, the Matérn 5/2 performance still outperforms others, though its performance is comparable to that of the MK approach.

5. Concluding Remarks

In this paper, we present the MK approach to improve kriging performance for complex problems. The MK approach assigns a different kernel function in the kriging construction, to better represent the heterogeneity of the function. The results presented in this paper show that the kernel selection is problem-dependent. Accuracy improvement, however, is consistently observed when multiple kernels are used. While the MK approach outperforms the accuracy performance in most cases, it also incurs the highest computational efforts, especially for higher-dimensional problems. Further investigations are needed to optimize the kernel combination for the problem at hand.

References

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