EFFICIENT SURROGATE MODEL CONSTRUCTION FOR LARGE DATA SETS USING BAYESIAN LEARNING

Daigo Maruyama[1*], Stefan Görtz[1], Simon Coggon[2]

[1]DLR
Institute of Aerodynamics and Flow Technology
Lilienthalplatz 7, 38108 Braunschweig, Germany
{Daigo.Maruyama, Stefan.Goertz}@dlr.de

[2]Airbus Operations Limited
Pegasus House, Aerospace Avenue, Filton, Bristol, BS34 7PA, UK
Simon.Coggon@airbus.com

ABSTRACT

Surrogate models have become a popular choice to enable the inclusion of high-dimensional, physics-based computational models in time-critical processes such as design, optimization and uncertainty quantification. Among the vast amount of different surrogate modeling strategies Kriging is one of the most promising offering accurate and rapid predictions between given sample points. However, to capture the underlying high-dimensional system behavior for complex engineering tasks, such as computational fluid dynamics, thousands to millions of sample points might be necessary. Thus, the computational cost for constructing the Kriging model can no longer be neglected since it requires iteratively solving linear systems – each of complexity cubic proportional to the number of samples – during the so-called hyperparameter tuning.

In this work an efficient method for constructing Kriging models is proposed to mitigate the computational bottleneck caused by large data sets. Instead of working on the whole data set at once the samples are divided into subsets and a Bayesian learning strategy [1] is applied. Samples are partitioned in subsets each of them retaining the uniformity (low-discrepancy) of the initial data sets. The achieved reduction in computational cost is at least square proportional to the number of partitions and offers the potential of being cubic proportional when additionally solving the arising smaller linear systems in a parallel fashion.

Results are presented for an analytical test case and for a large aerodynamic data set which was computed using the DLR-TAU code [2]. After partitioning the data a drastic reduction of computational cost is achieved without barely any impact on the prediction accuracy. Moreover, the developed method can be extended for other kernelized regression models such as Radial Basis Function, Co-Kriging and gradient-enhanced Kriging (GEK) [3,4]. Especially GEK shows excellent compatibility with the proposed method once an adjoint solver [2] is available. Overall, the bottleneck of the huge computational cost needed during the model construction for the hyperparameter tuning can be drastically decreased by the presented Bayesian learning strategy.

References

[1] C.M. Bishop, Pattern Recognition and Machine Learning (information science and statistics). Springer, 2007.
[2] D. Schwamborn, T. Gerhold, R. Heinrich, The DLR TAU-code: Recent applications in research and industry, invited lecture, in: P. Wesseling, E. Oate, J. Priaux (Eds.), Proceedings of the European Conference on Computational Fluid Dynamics (ECCOMAS CFD 2006), The Netherlands, 2006.
[3] Z.H. Han, S. Görtz, R. Zimmermann, Improving Variable-Fidelity Surrogate modeling via Gradient-Enhanced Kriging and a Generalized hybrid Bridge Function. Journal of Aerospace Science and Technology, Vol. 25, Issue 1. 2013.
[4] Z.H. Han, Y. Zhang, C.X. Song, K.S. Zhang, Weighted Gradient-Enhanced Kriging for High-Dimensional Surrogate Modeling and Design Optimization. AIAA Journal, Vol. 55, No 12. 2017.