Analyzing and Optimizing Expensive Computer Simulations: The Surrogate Model Approach

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Abstract. The analysis and design of complex engineering systems is a challenging task. While computing power is steadily increasing, the complexity of the simulation codes continues to keep pace. Accurate physics-based simulations can take hours to complete [3]. Often a scalable surrogate model is constructed based on high fidelity simulation data which can later be used for design and other tasks. Consequently, there is great interest in techniques that facilitate the construction and evaluation of such approximation models, while minimizing the computational cost and maximizing model accuracy. We present a novel, unified approach to surrogate modeling, placing a strong focus on adaptivity, self-tuning and robustness in order to maximize efficiency. Furthermore, substantial effort is put in making our algorithms and tools easily accessible to other scientists in computational science and engineering [1]. Besides constructing accurate surrogate models that approximate the global behavior of the simulator, rough, local surrogate models are often used in optimization methods. While optimization can also be applied in a post-processing step, it is often more economical to guide the selection of new simulation data samples directly towards the optimum. Efficient Global Optimization (EGO) [2], also called Sequential Kriging, is such a method that maximizes the information retrieved from the local surrogate model to determine the global optimum.

References

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