

Large-scale Constrained Black-box Optimization: Theory, Methodology and Applications

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Abstract: Black box optimization concerns the optimization of functions that can only be evaluated through numerical simulation and in which partial derivatives are either not known or not defined. One way to optimize these functions consists of using consecutive function evaluations to build and refine a surrogate model, and then use this model to drive the optimization. Albeit very effective, this model-based approach is typically computationally expensive, becoming impractical when the number of input variables is greater than just a few dozens. Moreover, it usually applies only to functions defined in bound-constrained feasible regions, i.e. hyperrectangles. These two aspects prevent this approach to be used on many relevant optimization problems.

We introduce innovative algorithms and methodologies to overcome these limitations. In particular, we first present a new sampling method that let us generate well-distributed samples (also called space-filling designs) within mixed-integer feasible regions. Secondly, we discuss an efficient implementation of a model-based approach that exploits a combination of Radial Basis Functions (RBF) approximation and scalable optimization methods to reduce the computation time. The resulting algorithm can handle black box optimization problems with up to few thousands variables and any mixed-integer feasible region. Moreover, we introduce an early optimization methodology that let us build and exploit a RBF model after just few function evaluations, a significant improvement compared to similar state-of-the-art RBF methods and a crucial development when the function evaluations are computationally expensive.

Finally, we apply our model-based black box optimization algorithm to the feature selection problem in machine learning and to the influence maximization problem in complex networks, reporting promising results.

Speaker Bio: Giorgio holds a Bachelor's degree in Information Engineering from University of Padua (2010) and a Master's degree in Automation Engineering from the same university (2012). He worked as a Research Assistant at the University of Padua before joining SUTD in 2013. Supported by the President's Graduate Fellowship, Giorgio is currently completing the PhD program in the ESD pillar. In 2015, he started collaborating with the IBM Singapore Research Lab. He is mainly interested in mathematical programming and machine learning, with a particular focus on developing innovative optimization techniques to solve black box problems.

