Automating Scientific Work in Optimization

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In the fields of heuristic optimization and machine learning, experimentation is the way to assess the performance of an algorithm setup and the hardness of problems. Good experimentation is complicated. Most algorithms in the domain are anytime algorithms, meaning they can improve their approximation quality over time. This means that one algorithm may initially perform better than another one but converge to worse solutions in the end. Instead of single final results, the whole runtime behavior of algorithms needs to be compared (and runtime may be measured in multiple ways). We do not just want to know which algorithm performs best and which problem is the hardest — a researcher wants to know *why*. We introduce a process which can *1)* automatically model the progress of algorithm setups on different problem instances based on data collected in experiments, *2)* use these models to discover clusters of algorithm (or problem instance) behaviors, and *3)* propose reasons why a certain algorithm setup (or problem instance) belongs to a certain algorithm (or problem instance) behavior cluster. These high-level conclusions are presented in form of decision trees relating algorithm parameters (or instance features) to cluster ids. We emphasize the duality of analyzing algorithm setups and problem instances. Our process is implemented as open source software and tested in two case studies, on the Maximum Satisfiability Problem and the Traveling Salesman Problem. Besides its basic application to raw experimental data, yielding clusters and explanations of "quantitative" algorithm behavior, our process also allows for "qualitative" conclusions by feeding it with data which is normalized with problem features or algorithm parameters. It can also be applied recursively, e.g., to further investigate the behavior of the algorithms in the cluster with the best-performing setups on the problem instances belonging to the cluster of hardest instances. Both use cases are investigated in the case studies.

Prof. Dr. Thomas Weise [汤卫思] obtained his *Diplom Informatiker* (Master of Computer Science) in 2005 from the Chemnitz University of Technology and his PhD from the University of Kassel in 2009. He then joined the University of Science and Technology of China [USTC, 中国科学技术大学] as PostDoc. The USTC is one of the top-three universities in China. Dr. Weise was promoted to Associate Professor at the USTC-Birmingham Joint Research Institute in Intelligent Computation and Its Applications (UBRI) at USTC in 2011. In 2016, he joined Hefei University as Full Professor to found the *Institute of Applied Optimization* [应用优化研究所] at the Faculty of Computer Science and Technology. Prof. Weise has more than 80 scientific publications in international peer reviewed journals and conferences. His book "*Global Optimization Algorithms – Theory and Application*" has been cited more than 850 times and he has acted as reviewer, editor, or programme committee member at 70 different venues. He has obtained funding from competitive national Chinese sources such as the Chinese National Natural Science Foundation [国家自然科学基金委员会], the Chinese Academy of Sciences [中国科学院], and the China Postdoctoral Science Foundation [中国博士后科学基金会]. He has supervised several graduate and undergraduate students.