Assessing Basin Identification Methods for Locating Multiple Optima

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Two-stage algorithms for global optimization are meta-heuristics consisting of a global and a local stage, which are executed alternatingly [3, p. 14]. The global stage is responsible for exploration, the local one for exploitation. The local stage is usually understood as a local search algorithm started at a certain point and running until convergence is detected. As this is quite expensive in terms of function evaluations, the global stage ideally has the capability of carefully selecting promising starting points [3, p. 66]. This task shall be denoted *basin identification*. Originally, it was accomplished by conventional clustering methods [3, pp. 95–116], but nowadays more refined methods have been developed, which are not necessarily clustering methods in a strict sense anymore [2].

In this work, we directly compare two basin identification methods regarding their ability to detect distinct attraction basins. Correspondingly, the task of approximating all or at least several local optima of a multimodal objective function in one optimization run has received increased attention of the optimization community in recent years. It is clear that the aim of finding, say, the best k optima is only a slight shift in perspective, as global optimization can be viewed as a special case of multimodal optimization. This change in perspective may be partly due to the rise of a-posteriori approaches for multiobjective optimization, where it is considered a critical property of the algorithms that they are able to generate whole Pareto front approximations, and it is left to the user to finally choose one of the available solutions. In order to enable an informed decision, it was already argued in [1] that alternative solutions in the search space are valuable in multiobjective optimization, even if one point in objective space has been selected. The same argument may be utilized for multimodal optimization, such that one wants to obtain the set of best solutions not only for finding the global optimum therein but also to have alternatives at hand when the seemingly best solution cannot be implemented.

In this work, we compare two approaches on their own, namely topographical selection and nearest-better clustering, regarding their ability to identify the distinct attraction basins of multimodal functions. We show that both have different strengths and weaknesses, as their behavior is very dependent on the problem instance. Thus, we try to build regression models on experimental data to predict appropriate parameter values based on the dimension and the number of points in the sample. We admit that the resulting prediction models are still very rough and somewhat depend on the number of optima employed in the experiments. However, we think the relatively low values chosen by us for this parameter correspond to a realistic application scenario.

Additionally, we repeat the recommendation to always use a sampling as uniform as possible, because this increases the precision of the basin identification. By using a more expensive sampling algorithm, such as maximin reconstruction, it is possible to further improve the performance as against quasirandom sequences. If it is not possible to control the sampling, a basin identification method robust to outliers must be sought.

References

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