Multi-objective Bayesian global optimization for continuous problems and applications

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English Summary

Evolutionary algorithms (EAs) and *Bayesian Global Optimization* (BGO) are two main branches in the field of multi-objective optimization. The first is based on the paradigm of encoding natural evolution for computational observation; the latter uses statistical models in optimization. However, in the field of multi-objective optimization, evolutionary multi-objective optimization algorithm (EMOA) approach as commonly used requires a large number of objective function evaluations and therefore is inefficient when dealing with expensive function evaluation problems. This problem can be solved by using the efficient method of Bayesian Global Optimization. When applying this method in multi-objective optimization, we have a new challenge to meet: the execution time of *multi-objective Bayesian Global Optimization* (MOBGO) itself is still too long, even though it only requires a few function evaluations. The reason for the high cost of MOBGO is two-fold: on the one hand, MOBGO requires an infill criterion to be calculated many times, but the computational complexity of an infill criterion has so far been very high. Another reason is that the optimizer, which aims at searching for an optimal solution according to the surrogate models, is not sufficiently effective.

For the aim of improving the performance of one of the most common infill criteria, *Expected Hypervolume Improvement* (EHVI), a new efficient algorithm is proposed in this thesis. This new efficient algorithm is based on an efficient partitioning algorithm for the non-dominated space and on a newly derived EHVI calculation formula. The computational complexity of the proposed algorithm for exact EHVI calculation is $O(n \log n)$ both in the cases of two and three objectives. It is shown that this time complexity can no longer be improved. In the case of three objectives, the execution time of the new algorithm is nearly forty thousand times faster than that of the previous algorithm. Moreover, this algorithm can also be extended for other exact calculations of infill criteria, for instance, *Probability of Improvement* (PoI) and *Truncated Expected Hypervolume*

Improvement (TEHVI).

To make full use of a-priori knowledge of objective functions, whenever it is available, TEHVI is proposed as a new infill criterion in this thesis. In the definition of TEHVI, the *probability density function* follows a truncated normal distribution, where the truncated domain is determined by the range of the objective functions. The exact calculation of TEHVI is derived from that of EHVI and the computational complexity of TEHVI is $O(n \log n)$ in the case of two objectives. Since the TEHVI is non-zero only in the valid truncated domain, it can lead the optimizer to the valid domain in the objective space for the aim of searching for the optimal solution. Therefore, compared to EHVI, the TEHVI can generate a better Pareto-front approximation. Moreover, the TEHVI can be utilized to solve the preference-based multi-objective optimization problems, when the truncated domain is set to be the preferred-region in the objective space.

To improve the effectiveness of the optimizer in MOBGO, another infill criterion, namely, Expected Hypervolume Improvement Gradient (EHVIG), is introduced in this thesis. EHVIG is the gradient of EHVI, which makes it possible to apply a gradient ascent algorithm, instead of an EA, in MOBGO as the optimizer. However, a well-known drawback of a gradient ascent (descent) algorithm is that it can easily get stuck at a local optimal solution. This problem is solved in this thesis by introducing the EHVIG as a new stopping criterion in an EA. The basic idea of this method is straightforward: once the EHVIG of one individual in an EA is very close to or even equal to a zero vector, this individual can be regarded as the optimal solution and it becomes unnecessary to continue the following iterations in the EA.

In this thesis, both state-of-the-art EMOAs (NSGA-II and SMS-EMOA) and MOBGO based algorithms are implemented and compared in different practical applications. These applications include the PID parameter tuning problems, the robust PID parameter tuning problems with disturbance, and the bio-gas plant optimization problems. In view of the better performance of the MOBGO based algorithms, it is recommended to use TEHVI-EGO and EHVI-EGO in practical applications.