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Multi-objective Bayesian global optimization for continuous problems and applications

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Chapter 1

Introduction

1.1 Background

Optimization is a process of searching for the best solution from a set of available solutions. Single-objective optimization and multi-objective optimization are two main branches. They are distinguished with respect to the number of considered objective functions. Specifically, single-objective optimization considers one objective function, while multi-objective optimization (MOO) involves more than one objective function simultaneously.[1] An easy way to solve a multi-objective optimization problem is to convert it into single-objective optimization, by forming a weighted sum of all objective functions. This method is simple but not effective when the objectives are conflict. This is the reason why researchers are interested in treating each objective separately and using the Pareto front concept for optimization.

Based on evolutionary algorithms, many evolutionary multi-objective optimization methodologies have been proposed over the past several decades in order to find an efficient approximation of the Pareto front. However, evolutionary multi-objective optimization (EMO) is inefficient when dealing with expensive function evaluation problems, because EMO usually needs more than ten thousand function evaluations and such a large number of function evaluations are unrealistic to be applied in many practical applications.

[1] In some papers, multi-objective optimization means the number of the objective functions is 2 or 3, and many-objective optimization is used to indicate more than 3 objective functions. Typically, optimization problems are defined by means of one or more objective function(s).

A common remedy to this problem is Multi-objective Bayesian global optimization (MOBGO), which partially replaces exact objective function evaluations by using predictions from the so-called Kriging or Gaussian process models. These surrogate models provide a predictive distribution, consisting of a mean value and a standard deviation of each objective function.[2] The scheme of a MOBGO involves sequentially updating the surrogate models by a predicted optimum and its corresponding objective function value. An optimizer is utilized in MOBGO in order to search for a predicted optimum, which is the next point for evaluation, according to the so-called infill criterion.

In practical applications, MOBGO is actually not widely utilized. This is because MOBGO requires a lot of execution time, even though it only requires far fewer evaluations of the objective functions. Three main aspects limit the efficiency of MOBGO:

1. Updating the surrogate models is very expensive;
2. Computational complexity of an infill criterion is very high;
3. The optimizer for searching an optimal solution from the surrogate models is not sufficiently effective.

To improve the efficiency and effectiveness of MOBGO, many researchers have attempted to overcome the drawbacks mentioned above. In order to update the surrogate models more efficiently, some researchers reduced the sampling data by using a clustering method. In this dissertation, the central research questions are surrounding the second and the third aspects to improve the performance of MOBGO.

1.2 Research Questions

The first research question of this work is how to improve the efficiency of exact EHVI calculation. Since an infill criterion plays an important selecting role in MOBGO and values the performance of the Pareto front approximation, it is essential to find an effective and efficient infill criterion in MOBGO. Some common infill criteria are *Hypervolume* (HV), *Hypervolume Improvement* (HVI), *Probability of Improvement* (PoI), *Expected Hypervolume Improvement* (EHVI). Compared to other criteria, EHVI takes the predictive mean value and

[2]The hypothesis of MOBGO is that objective functions are independent.

standard deviation into account and can balance exploitation[1] and exploration[1] well, which are two important aspects in optimization. Nevertheless, EHVI is mainly utilized in scientific research but seldom applied in real applications, which is caused by its high computational complexity. In order to solve this problem, an efficient EHVI calculation algorithm is proposed in this dissertation.

The second research question of this work is how to improve the effectiveness of MOBGO, by taking a-priori knowledge of the objective functions into consideration. The definition of EHVI is based on the concept of a normal distribution, with the assumption that an objective function value is a real number, from minus infinity to infinity. The EHVI assumes an unbounded objective space even if it is often known a-priori that the objective function values are within a prescribed range. In some cases, a-priori knowledge of the range of an objective function value is already available. For instance, in a PID[1] parameter tuning problem, the rising time is always a positive value. In these cases, it is assumed that surrogate-model based algorithms could converge to true Pareto front faster, if the range of the objective functions could be applied during the optimization. To take advantage of such a-priori knowledge, a new criterion called *Truncated Expected Hypervolume Improvement* (TEHVI) is proposed in this dissertation.

The third research question of this work is how to solve the preference-based Pareto front problems. In a practical application, what interests a decision maker (DM) is not the entire Pareto front approximation set, but how to find more solutions which can best match his/her preferences. TEHVI is capable of solving the preference-based Pareto front problems by setting the domain of the truncated normal distributions according to a decision maker's preference. Inspired by the concept of TEHVI, *Truncated Hypervolume* is also applied to solve this problem.

The last research question of this work is how to improve the efficiency of the optimizer in MOBGO. An optimizer searches for the optimal solution according to an infill criterion, which is based on the predictions of the surrogate models. Theoretically, any single-objective optimization algorithm can be applied as the optimizer in MOBGO. Usually, some state-of-the-art single-objective evolutionary algorithms are chosen for the optimizer, such as genetic algorithm (GA) and covariance matrix adaptation evolution strategy (CMA-ES). However,

[1]Exploitation means to search a limited but promising region in the search space.

[1]Exploration means to search a much larger region of the search space, with the hope of finding other promising solutions.

[1]PID controller is short for the proportional-integral-derivative controller.

EAs requires a large number of function evaluations of the infill criterion, in order to find the optimal solution and update the surrogate models. Because of this reason, MOBGO still requires much more execution time than evolutionary multi-objective optimization algorithms (EMOAs), even though MOBGO needs far fewer evaluations than EMOAs. To improve the efficiency of MOBGO, a new criterion called *Expected Hypervolume Improvement Gradient* (EHVIG) is utilized in an optimizer.

1.3 Dissertation Outline

The outline of this dissertation is described in this section. Each chapter of this dissertation is based on at least one publication of the author. The following provides a brief outline of each chapter.

- Chapter 2 lays out the definition of the multi-objective optimization problem and the terminologies used in this dissertation. A brief introduction of evolutionary multi-objective algorithms (EMOAs) is provided. These EMOAs are illustrated by a real application problem. Moreover, a brief introduction of Bayesian Global Optimization is also described, including a brief example to illustrate how MOBGO works. Parts of the definitions are previously published in [1, 2, 3]:

  Hupkens, I., Deutz, A., **Yang, K.**, Emmerich, M. (2015). Faster Exact Algorithms for Computing Expected Hypervolume Improvement. In: Gaspar-Cunha A., Henggeler Antunes C., Coello C. (Eds.), Evolutionary Multi-Criterion Optimization. EMO 2015. Lecture Notes in Computer Science, vol 9019. Springer, pp. 65-79, Cham.

  Emerich, M., **Yang, K.**, Deutz, A., Wang, H., Fonseca, M. (2016). Multicriteria generalization of Bayesian global optimization. In: Pardalos, P., Zhigljavsky, A., Žilinskas, J. (Eds.), Advances in Stochastic and Global Optimization. Springer, pp. 223-236.

  Yang, K., Emmerich, M.T.M., Li, R., Wang, J., Bäck, T. (2014). Power Distribution Network Reconfiguration by Evolutionary Integer Programming. In: Bartz-Beielstein T., Branke J., Filipič B., Smith J. (Eds.), Parallel Problem Solving from Nature–PPSN XIII. PPSN 2014. Lecture Notes in Computer Science, vol 8672, pp. 11-23. Springer, Cham.

- Chapter 3 defines what is *Expected Hypervolume Improvement* (EHVI) and how to calculate EHVI efficiently. The computational complexity of EHVI is analyzed, together with a comparison between the performance of EHVI and other infill criteria. Parts of this chapter are published in the following articles [4, 5]:

  Yang, K., Emmerich, M., Deutz, A., Fonseca, C.M. (2017). Computing 3-D Expected Hypervolume Improvement and Related Integrals in Asymptotically Optimal Time. In: Trautmann H. et al. (Eds.), Evolutionary Multi-Criterion Optimization. EMO 2017. Lecture Notes in Computer Science, vol 10173. Springer, pp. 685-700, Cham.

  Yang, K., Deutz, A., Fonseca, C.M., Bäck, T., Emmerich, M. (2017). Efficient exact computation of expected hypervolume improvement in Bayesian global optimization. Journal of Global Optimization, Submitted.

- Chapter 4 describes the definition and the exact calculation method of *Truncated Expected Hypervolume Improvement* (TEHVI). TEHVI is derived from the definition of EHVI, which utilizes the a-priori knowledge of the objective functions, in order to improve the efficiency of MOBGO, by means of the conditional distribution. Part of this chapter is published in the following article [6]:

  Yang, K., Deutz, A., Yang, Z., Bäck, T., Emmerich, M. (2016). Truncated expected hypervolume improvement: Exact computation and application. In: 2016 IEEE Congress on Evolutionary Computation (CEC), pp. 4350-4357, IEEE.

- Chapter 5 introduces preference-based multi-objective optimization. This chapter aims at finding a more fine-grained resolution of a preferred region, instead of exploring the whole set of Pareto front solutions. Two methods are applied in this chapter: TEHVI assisted by Bayesian global optimization and *Truncated Hypervolume* assisted by EAs. The works are previously published in [7, 8]:

  Yang, K., Li, L., Deutz, A., Bäck, T., Emmerich, M. (2016). Preference-based multiobjective optimization using truncated expected hypervolume improvement. In: 2016 12th International Conference on Natural Computation, Fuzzy Systems and Knowledge Discovery (ICNC-FSKD), pp. 276-281, IEEE.

  Wang, Y., Li, L., **Yang, K.**, Emmerich, M. (2017). A new approach to target region based multiobjective evolutionary algorithms. In: 2017 IEEE Congress on Evolutionary Computation (CEC), pp. 1757-1764, IEEE.

- Chapter 6 proposes a new infill criterion, namely, the gradient of EHVI (EHVIG) and utilizes EHVIG in multi-objective optimization by two approaches: one is applying EHVIG in gradient ascent algorithm and the other is regarding EHVIG as a stopping criterion in evolutionary algorithms to find the globally optimal solution. This work is mainly in the following paper [9]:

  Yang, K., Emmerich, M., Bäck, T., Deutz, A. (2017). Multi-objective Bayesian global optimization using expected hypervolume improvement gradient. Swarm and Evolutionary Computation, Submitted.

- Chapter 7 mainly concerns real-world applications of multi-objective optimization, particularly in the fields of bio-gas plant and PID parameter tuning. These works have been previously published in [6, 10]:

  Yang, K., Gaida, D., Bäck, T., Emmerich, M. (2015). Expected hypervolume improvement algorithm for PID controller tuning and the multiobjective dynamical control of a biogas plant. In: 2015 IEEE Congress on Evolutionary Computation (CEC), pp. 1934-1942, IEEE.

  Yang, K., Deutz, A., Yang, Z., Bäck, T., Emmerich, M. (2016). Truncated expected hypervolume improvement: Exact computation and application. In: 2016 IEEE Congress on Evolutionary Computation (CEC), pp. 4350-4357, IEEE.

- Chapter 8 summarizes the contribution of this dissertation and provides some suggestions for future work.

- Besides the publications mentioned above, other publications of the author is [11]:

  Yang, Z., Wang, H., **Yang, K.**, Bäck, T., Emmerich, M. (2016). SMS-EMOA with multiple dynamic reference points. In: 2016 12th International Conference on Natural Computation, Fuzzy Systems and Knowledge Discovery (ICNC-FSKD), pp. 282-288, IEEE.