A Stopping Criterion for Surrogate Based Optimization using EGO

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Abstract

In Surrogate-based optimization, each optimization cycle consists of fitting a surrogate to a number of simulations at a set of design points, and performing optimization based on the surrogate to obtain one or more new design points. Algorithms like Efficient Global Optimization (EGO) [1] use uncertainty estimates available with the Kriging surrogate to guide the selection of new point(s). The most common EGO variant uses prediction and prediction variance to seek the point of maximum Expected Improvement (EI) [1] as the next point to be sampled in the optimization. A major problem in global optimization has been the lack of an adequate stopping criterion. The traditional goal of stopping criteria has been convergence to the optimum, but this is not practical when each cycle is expensive and convergence is slow.

There have been few stopping criteria proposed for surrogate based optimization algorithms. The number of objective function evaluations is a common stopping criterion. Schonlau proposed for EGO to stop if the maximum EI is below an absolute tolerance or the ratio of the maximum value of EI to the present best solution is below a relative tolerance [1]. When each cycle of surrogate based optimization is very expensive or time consuming, we may not afford to proceed, even while being far from the global optimum. One practical question when considering whether to stop or carry out one more cycle is whether the resources invested in this additional cycle would yield sufficient return to justify it.

In this paper we propose a stopping criterion which justifies continuing with one more cycle only if it is expected to yield at least a specified improvement in the objective function. To implement this stopping criterion the most common EGO variant with EI is used along with a specified improvement that makes it worthy to continue with the optimization, based on a criterion suggested by Schonlau [1]. Its efficiency is also compared to a case using a variant of EGO which uses Probability of targeted Improvement (PI) with an adaptive target, EGO-AT [2]. EGO-AT provides two important ingredients for the criterion: (i) a reasonable target for improvement in the next cycle, and (ii) the probability of achieving that target. The effectiveness of the stopping criteria for both algorithms is demonstrated using a few benchmark global optimization problems.

References

[1] Jones D, Schonlau M, and Welch W, "Efficient global optimization of expensive black-box functions," *Journal of Global Optimization,* Vol. 13 (4), pp. 455-492, 1998.

[2] Chaudhuri A, Haftka RT, Viana FAC, "Efficient Global optimization with adaptive target for Probability of target Improvement," *8th AIAA Multidisciplinary Design Optimization Specialist Conference*, Honolulu, USA, April 23-26, 2012.