Optimal and sub-optimal stopping rules for the Multistart algorithm in global optimization

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In this paper the problem of stopping the Multistart algorithm for global optimization is considered. The algorithm consists of repeatedly performing local searches from randomly generated starting points. The crucial point in this algorithmic scheme is the development of a stopping criterion; the approach analyzed in this paper consists in stopping the sequential sampling as soon as a measure of the trade-off between the cost of further local searches is greater than the expected benefit, i.e. the possibility of discovering a better optimum.

Stopping rules are thoroughly investigated both from a theoretical point of view and from a computational one via extensive simulation. This latter clearly shows that the simple 1-step look ahead rule may achieve surprisingly good results in terms of computational cost vs. final accuracy.

Key words: Global optimization.

Introduction

In Betrò and Schoen (1987) the problem has been considered of developing suitable stopping rules for the Multistart algorithm in global optimization. Such a problem was seen as a problem of sequential decision under uncertainty and thereafter a stochastic model for the observations (sampled extrema) and a cost connected with sampling were introduced. In order to circumvent the difficulties of deriving optimal stopping rules, i.e., rules which attain the minimum expected cost at stopping, suboptimal rules of the 1- and 2-step look-ahead (sla) type were obtained. Although the results presented were encouraging, confirmed by the simulations presented in Betrò and Schoen (1991), several questions arise concerning the practical behavior of the proposed rules. The first question is related to the relative performance of the 1-sla and the 2-sla rules; indeed it was observed that the costs evaluated at the

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stopping times of the two rules are very close, so that the convenience of the 2-sla in comparison with the much simpler 1-sla is questionable. The second question is whether the two rules, whose expected costs are necessarily larger than that of an optimal one, are close to this latter or not. Unfortunately, under the adopted stochastic model it is impossible to obtain close information about the expected cost of the optimal stopping rule, so the answer to this question is not easy. The third question is obviously whether the stochastic model is an appropriate one, that is whether rules obtained under it, even optimal, are indeed good rules for actual situations. In the light of the above questions, the purpose of this paper is to carry out further investigation about the behavior of the 1- and 2-sla rules. In Section 1 the decision theoretic approach, proposed in Betrò and Schoen (1987) for the problem of stopping the Multistart algorithm, is recalled; the approach is shown to lead to the problem known in the literature as the problem of optimal sampling with recall. In Section 2 some analytical considerations are derived concerning the behavior of the 1- and 2-sla stopping rules; in Section 3 the results of an extensive simulation study of such behavior are presented and discussed.

1. Optimal stopping of the Multistart algorithm

The problem of finding a global optimum of a real-valued function can be stated as follows:

$$\max_{x \in K} f(x), \quad K \subseteq \mathbb{R}^k, \quad k \geq 1, \quad (1)$$

where $f$ is assumed to be continuous and $K$ compact. A very simple, yet attractive algorithm for problem (1) is the so-called Multistart algorithm, which consists in sequentially performing local optimizations from randomly chosen starting points. The algorithm obviously will eventually succeed in locating the global optimum (with probability 1); a crucial point is the decision at each step whether to stop or continue performing local optimizations. Effective solutions to this decision problem can be looked for only after the introduction of a model capable of taking into account the trade-off between the cost connected with performing more local searches and the (expected) benefit coming from the possible discovery of a new local optimum. In Boender and Rinnooy Kan (1987), following ideas introduced in Zieliński (1981), a Bayesian decision-theoretic framework was introduced in which a cost structure is imposed over the problem, associating a penalty for stopping before all of the local optima, and hence a fortiori the global one, have been observed. While this approach leads to quite simple stopping criteria, it does not take into account the values of the objective function at the local optima; this leads to wasting relevant information about the function itself gathered during the local searches, while gaining information about not yet discovered, but perhaps not interesting, local optima. It has to be observed that this drawback has been recently partially overcome in Piccioni and Ramponi (1990).