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A peak-over-threshold search method for global optimization☆

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ABSTRACT

In this paper, we propose a random search method, called peak-over-threshold search (POTS), for solving global optimization problems. An important feature of POTS is that it combines the existing partition-based random search framework (e.g., Shi and Ólafsson 2000a; Chen et al. 2011) with the peak-over-threshold statistical reference (Coles, 2001) in order to achieve high search efficiency. In each iteration, POTS partitions the solution space into several subregions, evaluates the quality of each subregion and moves to promising subregions for more partitioning and sampling. To effectively assess the quality of a subregion, an extreme value type of inference in statistics is used to develop a new promising index which reflects the optimal objective value of a subregion and biases the search to regions that are likely to contain the optimal or near-optimal solutions. Under assumptions on the depth of partitioning and the probability of correct movement, POTS is shown to converge with probability one to the optimal region. The higher efficiency of the proposed method is illustrated by numerical examples. The application of POTS to beam angle selection, an important optimization problem in radiation treatment, is also presented in this paper.
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1. Introduction

A variety of complex systems arising in control and engineering design applications require the use of optimization techniques to improve their performance. For example, in the problem of access and service rate control, we want to identify the rate design that minimizes the cost of the queueing systems, and in the Witsenhausen problem, a well-known problem in continuous-time optimal control, we want to find the control law that minimizes the expected cost function. However, for large-scale complex systems, these optimization problems can be extremely difficult to solve due to the large solution space, presence of multiple local optima and lack of structural properties. Due to the need for efficiency in solving these problems, metaheuristic algorithms, which aim to find good enough solutions instead of an optimal one, have drawn great attention. Although there is no guarantee for the solution quality, the metaheuristic algorithms can assert a certain degree of confidence about their performances "most of the time". Some well known metaheuristic algorithms are simulated annealing (SA) (Kirkpatrick, Gelatt, & Vecchi, 1983), genetic algorithm (GA) (Goldberg, 1989), tabu search (TS) (Glover, 1990), particle swarm optimization (PSO) (Kennedy & Eberhart, 1995) and ant colony optimization (ACO) (Dorigo, Caro, & Gambardella, 1999).

There is an important class of methods in metaheuristic algorithms which tackle the complex and encompassing situations of large-scale optimization using the idea of partitioning, called *partition-based random search* (PRS). PRS partitions the solution space into several small subregions and concentrates the computing effort in regions that are more promising. The most representative partition-based random search algorithms include nested partitions (NP) method (Chen, Pi, & Shi, 2009, 2011; Shi & Ólafsson, 2000a), adaptive partitioned random search (APRS) (Tang, 1994), partition-based lookahead algorithm (Linz, Huang, & Zabinsky, 2015), etc. PRS is also related to the branch-and-bound method (Horst, 1986) in mathematical optimization. The high efficiency of the PRS method has been discussed in detail in Tang (1994).

A typical PRS algorithm involves the following components.

- Partitioning of the solution space into smaller subregions.
- Sampling that randomly draws feasible solutions and evaluates the objective function at these points.
- Estimating the promising index of each subregion. The promising index reflects how good the subregion is.

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- Moving to the most promising region for further partitioning and sampling. The most promising region is usually the subregion with the best promising index.

From the optimization perspective, the promising index of a region should ideally be the objective value of the optimal solution in that region. The most promising region is then the subregion containing the global optimum. It is the region that deserves more computing effort. In a PRS procedure, whether the promising index can be accurately estimated is critical. It determines whether the algorithm can correctly recognize the promising regions and move there for more partitioning and sampling. Chen et al. (2009, 2011) and Tang (1994) assessed the promising index of a region using expected sample improvement, linear relaxation and solution value prediction respectively. Nevertheless, none of them represent the optimal objective value of the region. Shi and Ólafsson (2000a) used the objective value of the best sample point as an estimate for the promising index. Although this estimate converges to the optimal objective value as the sample size increases, it does not use the sample efficiently, because in addition to the best single sample point, the near-best sample points also provide a lot of information on the optimal objective value.

Assessing the promising index of a region is, in a sense, seeking the extreme value of the set of solution values in the region, based on a partial observation of the set. It is closely related to a line of research in statistics, which aims at making statistical inferences on extreme phenomena through available samples. Such statistical inferences provide theoretical support for the estimation of the promising index and are more reliable than some intuition-driven estimation heuristics. A broadly studied approach along this line that addresses the need for extremum modeling is the *peak-over-threshold* (POT) model (Coles, 2001). POT is a modern technique and can be seen as an extension of the traditional extreme value theory (EVT). It sets a threshold for samples and constructs a generalized Pareto distribution (GPD) for those samples over (or under) the threshold. Applications of POT are seen in many research fields like meteorology, hydrology, oceanography, geothermic, finance, management, logistics, biomedicine, food science, etc. To the best of our knowledge, however, the possibility of applying POT to optimization algorithms to guide the search for global optimum was seldom explored.

In this paper, we propose a PRS type of randomized method, called *peak-over-threshold search* (POTS), for global optimization. POTS inherits the basic characters of PRS algorithms, which systematically and iteratively partition the solution space and move to the promising areas. To correctly and effectively evaluate and compare each subregion, POTS uses the POT model for statistical reference. The motivation behind this method is to take advantage of the partitioning technique to improve sampling utility while enhancing via statistical tools the critical step of subregion quality evaluation and comparison in PRS. By utilizing statistical inference, we believe POTS can be an efficient and powerful metaheuristic algorithm.

Our main contributions are threefold. (1) We introduce an effective PRS-type framework for global optimization, which embeds statistical information into the optimization procedure to guide the search for global optimum. (2) A new and effective promising index is developed using the peak-over-threshold model to assess the extreme value of a region. (3) For beam angle selection, a very important combinatorial optimization problem in radiation treatment, POTS significantly improves the clinical plans for four cancer cases.

The remainder of the paper is organized as follows. In Section 2, we introduce the POT model, develop the POT promising index and design the POTS algorithm. In Section 3, we discuss the accuracy of the POT promising index estimator and the convergence of the POTS algorithm. Section 4 provides numerical examples, which demonstrate the claimed benefits of the proposed method. Finally, Section 5 concludes the paper.

2. Peak-over-threshold search

In this research, we consider problems of the following form:

$$x^* \in \arg\min_{x\in\Theta} f(x), \tag{1}$$

where the non-empty solution space Θ is bounded in $\mathbb{R}^n$. The objective function $f : \Theta \to \mathbb{R}$ is continuous. There are no linearity or convexity requirements imposed on f except that it is bounded from below. Throughout this paper, we assume that problem (1) has a unique global optimum.

2.1. Peak-over-threshold model

POT was originally designed for exceedance over a threshold but can be equivalently adapted to exceedance under a threshold (Pickands, 1975). Since in this paper we are discussing minimization, we will use the under-threshold version of POT.

Let $Y_1, Y_2, \ldots, Y_k$ be a sequence of independent and identically distributed (i.i.d.) random variables having common distribution function F and Y be an arbitrary term in the $\{Y_i\}$ sequence. The POT model tells us that for a low enough threshold u, the random variable $u - Y$, conditional on $Y < u$, approximately follows a generalized Pareto distribution (GPD) as $k \to \infty$. Theoretical justification of GPD approximation is given by Pickands (1975).

GPD is a two-parameter family of distributions with cumulative distribution function (c.d.f.) $G(y)$ being $1-(1+\frac{\xi y}{\sigma})^{-\frac{1}{\xi}}$ if $\xi \neq 0$ and $1-\exp(-\frac{y}{\sigma})$ if $\xi = 0$. σ and ξ are the scale and shape parameters ($\sigma > 0$). The range for y is $y > 0$ if $\xi \geq 0$ and $0 < y < -\sigma/\xi$ if $\xi < 0$.

2.2. POT promising index

According to the POT model, $u - Y|Y < u$ has GPD distribution for an appropriate threshold u. If we see values of the sample points drawn from a region as a realization of a sequence of i.i.d. random variables, the GPD conclusion on $u - Y|Y < u$ offers important information about the performance of the best sample point that can be possibly reached in the long term.

To make use of POT, suppose that $y_1, y_2, \ldots, y_k$ are the objective values of sample points obtained in a region. We set a threshold u for them. Exceedance points are observed as $\{y_i : y_i < u, i = 1, 2, \ldots, k\}$, which correspond to sample point values exceeding u in quality. Relabel them as $\{z_j, j = 1, 2, \ldots, m\}$. Define threshold excesses by $s_j = u - z_j$ for $j = 1, 2, \ldots, m$. If the choice of u is appropriate, the behaviors of s_j for $j = 1, 2, \ldots, m$ can be fitted to $u - Y|Y < u$, which is GPD according to POT.

Recall (in Section 2.1) that the feasible region of a GPD c.d.f. $G(y)$ is bounded from above by $-\sigma/\xi$ if and only if $\xi < 0$. In our targeted problem (1), the objective function is bounded from below. That is, for a fixed threshold, the threshold excesses are bounded from above. Therefore, $\xi < 0$, and the corresponding upper extreme for threshold excesses is $-\sigma/\xi$. This extreme point suggests the highest threshold excess amount that can be possibly achieved. Then, $u - (-\sigma/\xi) = u + \sigma/\xi$ is the lowest point a solution value can possibly be in a region. It reflects the best objective value of this region. In this research, we let it be the promising index of the partition-based random search. By defining the promising index like this, we always bias our search effort in the subregion with the best objective value, i.e., the subregion that contains the global optimum.

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