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Visualization of a statistical approximation of the Pareto front

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ABSTRACT

A bi-objective optimization problem is considered assuming that the objective functions can be non-convex expensive black-box type functions. A statistical model based visualization method is proposed to aid a decision maker in selecting an appropriate trade-off between objectives in case of scarce available information.

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1. Introduction

A large variety of methods have been proposed for multi-objective optimization depending on the assumed properties of the considered problems. Some extended versions of classical mathematical programming methods have been proved very efficient for convex multi-objective problems [1,2]. Meta-heuristic algorithms, which gained popularity in the solution of single-objective applied optimization, including black-box global optimization, were successfully generalized for the solution of multi-objective optimization problems with similar unfavorable properties [2,3]. We aim in this paper at a subclass of the multi-objective optimization problems which still remains insufficiently researched. Namely, we consider a multi-objective optimization problem assuming that the objective functions can be non-convex, and moreover, that they are expensive black-box type functions. The generalized versions of classical mathematical programming methods are of limited applicability to the problems considered here because of non-convexity of objective functions. Meta-heuristic algorithms are also of limited applicability here since the objective functions are supposed expensive to evaluate.

One of the possible approaches to construct a suitable algorithm for the considered class of problems is to seek an optimal/rational exploitation of the scarce information available during the search for an appropriate solution. To construct a theoretically substantiated algorithm a mathematical model of the problem should be chosen. The Lipshitz function model is very popular in deterministic single-objective global optimization [4–9] . The other well developed direction in single-objective global optimization is based on statistical models [10–15]. These models and ideas were generalized to the multi-objective case, e.g. in [16,17]. The optimality property is of great interest from the theoretical point of view. Optimal algorithms are not always suitable for applications either because of the implementation complexity or because of the sensitivity to the accepted assumptions.

For the expensive black-box multi-objective optimization problems it seems reasonable to hybridize a computer aided algorithmic search with interactive human heuristics. Visualization is very important in perception of relevant information by a human expert [18–20]. In the present paper we investigate possibilities of the visualization of scarce information on the Pareto front using a statistical model of the considered problem.

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2. Problem statement

We consider the following problem of bi-objective optimization:

$$\min_{X \in \mathbf{A}} F(X), \quad F(X) = (f_1(X), f_2(X))^T, \tag{1}$$

where the properties of $F(X)$ and of the feasible region $\mathbf{A} \subseteq \mathbb{R}^d$ are specified later on. Theoretically the solution to problem (1) consists of two sets: $\mathbf{P}(F)_O$ - the Pareto optimal solutions in the space of objectives, and $\mathbf{P}(F)_D$ - Pareto optimal decisions in $\mathbf{A}$ [1]. Analytically these sets can be found only in very special cases. We are interested in the approximation and visualization of $\mathbf{P}(f)_O$ using scarce information obtained in the initial/exploration phase of optimization. The necessity of the exploration phase follows from the assumption on the black-box objectives. This assumption means that such unfavorable, from the point of view of the optimizer, properties as non-convexity, non-smoothness, and noise in available function values can not be excluded. The human heuristic abilities can be advantageous here in perception of scarce information gained during the exploration. The restriction of information scarcity is implied by the assumption on expensiveness of the objectives. The further search can be rationally planned by the optimizer depending on the results of the exploration. Visualization is expected to aid the perception of the available results.

3. Statistical model

The exploratory phase assumes that we have values of the objective functions at some number of random points in $\mathbf{A}$ which are independent and uniformly distributed. This exploration method can be seen as an analog of a popular heuristic decision by throwing a coin in the case of a very uncertain decision situation. Moreover, the uniform distribution of points in the feasible region is the worst-case optimal algorithm for the multi-objective optimization of Lipschitz objectives as shown in [17]. Although in the latter case the uniformity is understood in the deterministic sense, the random uniform distribution of points is a frequently used simply implementable approximation of the deterministic one. In order to guide further search we have to extract useful for further search information from the available data, i.e. from a set of $X_i,\ Y_i = F(X_i),\ i = 1, \ldots, n$.

In the single-objective global optimization, some information on the global minimum of $f(X)$ can be elicited from the sample $z_i = f(X_i)$, where X_i are independent random points, by means of the methods of statistics of extremes [14] and [15]. We cite below some results by Zhigljavsky [15] which we intend to adapt to the considered problem of visualization of the approximated Pareto front.

Let us consider a sample of independent identically distributed random variables $z_i,\ i = 1, \ldots, n$. Let $G(t)$ be the distribution function of the considered random variables, and $G(t) = 0,\ t \le z,\ G(t) > 0, t > z$, where z denotes the minimum value of $f(X)$. Under rather general assumptions on the class of functions $f(X)$ and on the distributions of X_i the following representation of $G(t)$ for $t \simeq Z$ is valid

$$G(t) = 1 - c(t - z)^{\alpha} + o((t - z)^{\alpha}), \quad t \downarrow z, \tag{2}$$

where $c > 0$, $\alpha > 0$. The constant α is called the 'tail index', and it depends on the behavior of $f(X)$ in the vicinity of the global minimizer. We will assume that α is known. For our further analysis the value of c is not important. Some estimators of Z for known α are presented, e.g. in [14], Secttion 2.4. Among these estimators, the optimal linear estimator based on the use of k order statistics is of special interest because of good asymptotic properties and because it is defined by the following simple formula:

$$\widehat{z}_{n,k} = c \sum_{i=1}^{k} [u_i / \Gamma(i + 2/\alpha)] z_{i,n}, \tag{3}$$

where $\Gamma(\cdot)$ is the Gamma-function, $z_{1,n} \le z_{2,n} \le \ldots \le z_{n,n}$ are the ordered statistics of the sample $z_i,\ i = 1, \ldots, n$, and

$$u_i = \begin{cases} (\alpha + 1), & \text{for } i = 1, \\ (\alpha - 1)\Gamma(i), & \text{for } i = 1, \ldots, k - 1, \\ (\alpha - \alpha k - 1)\Gamma(k), & \text{for } i = k, \end{cases}$$

$$1/c = \begin{cases} \sum_{i=1}^{k} 1/i, & \text{for } \alpha = 2, \\ \frac{1}{\alpha - 2}(\alpha \Gamma(k+1)/\Gamma(k + 2/\alpha) - 2/\Gamma(1 + 2/\alpha)), & \text{for } \alpha \neq 2. \end{cases}$$

The following confidence interval for z has asymptotic (as $n \to \infty$) confidence level $1 - \delta$:

$$[z_{1,n}, z_{1,n} - (z_{k,n} - z_{1,n})/c_{k,\delta}], \quad \text{where} \quad c_{k,\delta} = [1 - (1 - \delta)^{1/k}]^{-1/\alpha} - 1. \tag{4}$$

The presented estimator and confidence interval have been used in construction of single-objective global optimization algorithms and their stopping conditions [15]. In [22] this idea was extended to multi-objective optimization via scalarization of the multi-objective problems. In the present paper we apply a similar approach to the visualization of a statistical approximation of the Pareto front using a sample of values of the objective functions computed at random points.

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