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Aggregation Trees for visualization and dimension reduction in many-objective optimization

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A B S T R A C T

This paper introduces the concept of Aggregation Trees for the visualization of the results of high-dimensional multi-objective optimization problems, or many-objective problems and as a means of performing dimension reduction. The high dimensionality of many-objective optimization makes it difficult to represent the relationship between objectives and solutions in such problems and most approaches in the literature are based on the representation of solutions in lower dimensions. The method of Aggregation Trees proposed here is based on an iterative aggregation of objectives that are represented in a tree. The location of conflict is also calculated and represented on the tree. Thus, the tree can represent which objectives and groups of objectives are the most harmonic, what sort of conflict is present between groups of objectives, and which aggregations would be helpful in order to reduce the problem dimension.

1. Introduction

Real-world optimization problems often have many conflicting objectives and, as a consequence, multi-objective optimization problems have become a major field of research. Sometimes these problems can be solved by aggregating all of the objectives into a single objective function that gives some weight to each of the objectives. However, very often, it is more important to understand the relationship between the objectives in order to make decisions with a reasonable understanding of the trade-off involved among the possible choices.

When there are few objectives to be considered, evolutionary algorithms are usually suitable to find the best combination of solutions to a problem and it is not very difficult to represent that set of possibilities (Section 2). As the number of objectives grow, we reach the field of many-objective problems (Section 2.3). The optimization of these problems becomes more challenging as most solutions become incomparable as the Pareto dominance selection becomes less discriminating. That means that any solution in our set of candidates is almost always better than all other solutions for at least one specific combination of objective weights. Besides, representing quality for a set of solutions in this context is equally a problem.

In order to address this problem, we propose the concept of Aggregation Trees (Section 3). Aggregation Trees iteratively group objective functions in tree nodes according to their harmony (a concept mathematically defined in Section 4), similar

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to an agglomerative hierarchical clustering method. Thus, it represents the relationship between conflicting groups of objectives for a problem. It also represents the globality or locality of the conflict, the region of concentration of the calculated conflict (as mathematically defined in Section 5) through branch colors and it shows which is the best combination of objectives to be aggregated for dimension reduction.

The contributions of the proposed approach are:

- Visualization of results for many-objective problems including particularly:
  - The amount of harmony and conflict between relevant groups of objectives.
  - The globality or locality of the conflict.
  - The region where the conflict is more intense in the objective space, when conflict is not equally spread in the objective space.
- Representation of the most useful aggregations in order to iteratively perform dimensionality reduction on any number of objectives of the original problem.
- Robustness in relation to problems where the relationship between objectives is not linear. This is obtained by employing a non-parametric analysis.
- The position of nodes in the tree suggest convenient positions for the representation of absolute objective values in parallel coordinate plots.
- Polynomial computational cost and ease of implementation.

Thus, as the majority of solutions in many-objective problems tend to be non-dominated, Aggregation Trees can be used as a method for providing the decision maker with enough information to restrict the preference area for a problem, restrict the domain of search variables, create new constraints for the problem or reduce the number of objectives in a further analysis.

We describe the algorithm in Section 6, analyze the polynomial time complexity of the suggested method in Section 6.1, and apply it to test instances in Section 7. We then conclude our paper with discussions about the method and suggestions concerning possible future work (Section 8).

2. Historical perspective

Complex problems often require the consideration of many criteria of performance, and, as a consequence, multi-objective problems are a well studied topic in the scientific literature. In simple approaches, objectives are aggregated into a single objective function that takes into account the utility of each objective. However, in a multi-objective problem, the solution set can be found to represent the trade-off between those objectives [12,10,21]. The solutions that represent this compromise are in the Pareto-optimal set, which has only non-comparable optimal solutions in the objective space. This means that no solution in the Pareto-set is preferable to another in relation to all objectives.

2.1. Multi-objective optimization problems

Definition 2.1. A multi-objective optimization problem can be defined as:

$$\min(f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})), \ \mathbf{x} \in \mathcal{F} \tag{1}$$

where $\mathbf{x}$ is a solution for the problem and $f_i(\mathbf{x})$ is the i-th objective function to be minimized.

Each function $f_i(\mathbf{x})$ maps the optimization variables of a candidate solution $\mathbf{x}$ to an objective value represented in one dimension of the objective space, i.e., $f_i(\cdot) : \mathbb{R}^n \mapsto \mathbb{R}$.

Definition 2.2. The set of all combinations of possible values for optimization variables defines the search space $\mathcal{S}$:

$$\mathcal{S} = \{\mathbf{x} = \{(x_1, v_1), \ldots, (x_n, v_n)\} : v_i \in \mathcal{D}_i\} \tag{2}$$

where each variable x_i assumes the value v_i in its respective domain $\mathcal{D}_i$.

Definition 2.3. If the problem has constraints, those constraint functions $g_i(\mathbf{x}), i = 1, \ldots, r$ define the feasible set of solutions $\mathcal{F}$:

$$\mathcal{F} = \{\mathbf{x} \in \mathcal{S} : g_i(\mathbf{x}) \leqslant 0, i = 1, \ldots, r\} \tag{3}$$

In multi-objective problems, the comparison between solutions has to consider all objective functions. We can only say $\mathbf{x}^1$ is a better solution than $\mathbf{x}^2$ if $\mathbf{x}^1$ is better on all the objective functions.

Definition 2.4. Let $f(\mathbf{x}^1) \prec f(\mathbf{x}^2)$ denote that a feasible solution $\mathbf{x}^1 \in \mathcal{F}$ dominates another solution $\mathbf{x}^2 \in \mathcal{F}$. $f(\mathbf{x}^1) \prec f(\mathbf{x}^2)$ iff the conditions below are attained: