On the Interrelationships Between Knees and Aggregate Objective Functions

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ABSTRACT

Optimizing several objectives that are often at odds with each other provides difficult challenges that are not encountered if having only one goal at hand. One intuitive way to solve a multi-objective problem is to aggregate the objectives and reformulate it as an optimization problem having just a single goal. This goal can be a designer specific aggregation of the objectives or a characterization of knees, trade-offs, utilities, stronger optimality concepts or preferences.

This paper examines the theoretical relationships between two knee concepts and aggregate objective functions methods. The changes in the fitness landscape by utilizing different aggregations is also discussed.

Categories and Subject Descriptors

F.2 [**Theory of Computation**]: Analysis of Algorithms and Problem Complexity; F.m [**Theory of Computation**]: Miscellaneous

Keywords

Knees; weighted sum method; fitness landscape

1. INTRODUCTION

Given $\mathbf{f}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^m$ and $X \subseteq \mathbb{R}^n$, the multi-objective optimization problem (MOP) is defined as follows:

$$\min_{\mathbf{x}} \mathbf{f}(\mathbf{x}) := (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})) \qquad \text{s.t. } \mathbf{x} \in X.$$

A point $\mathbf{x}_p \in X$ is called *Pareto-optimal* if no $\mathbf{x} \in X$ exists so that $f_i(\mathbf{x}) \leq f_i(\mathbf{x}_p)$ for all indices i with strict inequality for at least one i. In this paper, we study in interrelationships between knees (the a priori interesting Pareto-optimal solutions) and weighted sum based aggregation techniques.

2. WEIGHTED SUM VS. UTILITY KNEE

The *utility knee* was introduced in [2] and is related to the weighted sum method, a common approach for transforming a multi-objective into a single-objective optimization problem by aggregating and weighing individual objective values. The approach draws its inspiration from utility theory and its application proposed by von Neumann and Morgenstern [7]. A linear utility function $U(\mathbf{x}, \lambda)$ to assess the desirability of a solution $\mathbf{x}$ can be defined as follows:

$$U(\mathbf{x}, \lambda) = \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) \qquad \text{s.t. } \sum_{i=1}^{m} \lambda_i = 1, \quad \lambda_i \geq 0. \quad (1)$$

As computing the utility for every possible weight vector is not practical, we use an approach, similar to the utility computation from [1], to calculate the utility of a point.

THEOREM 1. *Let Λ^m denote the set of all feasible weight vectors $\lambda := \{\lambda_1, \ldots, \lambda_m\}$ for m objectives that additionally satisfy $\sum_{i=1}^m \lambda_i = 1$ and $\lambda_i \geq 0$ for all $i \in \{1, \ldots, m\}$. The solution $\mathbf{x} \in X_p$ that has the minimum sum of objectives $\sum_{i=1}^m f_i(\mathbf{x})$ is the solution that has the minimum expected utility $\sum_{i=1}^m \lambda_i f_i(\mathbf{x})$ over all uniformally distributed $\lambda \in \Lambda^m$.*

From the perspective of utility theory, Theorem 1 implies that the solution that has the minimum overall sum of objective values should always be preferred. However, it does not imply that the utility knee always coincides with the point minimizing the sum of all objectives. How often a given solution is the best choice for a particular $\{\lambda^j\}$ depends mainly on the shape of the Pareto front and its density.

3. WEIGHTED SUM VS. PROPER KNEE

In [3–5], a concept to bound the tradeoff between individual objectives was introduced. The main idea is to bound the trade-offs by bound by a finite number M. By minimizing M, we move towards more desirable solutions. Let $I := \{1, 2, \ldots, m\}$, and, for any two vectors $\mathbf{x}, \mathbf{y} \in X$, $I_<(\mathbf{x}, \mathbf{y})$ and $I_>(\mathbf{x}, \mathbf{y})$ be defined by $I_<(\mathbf{x}, \mathbf{y}) := \{i \in I | f_i(\mathbf{x}) < f_i(\mathbf{y})\}$ and $I_>(\mathbf{x}, \mathbf{y}) := \{i \in I | f_i(\mathbf{x}) > f_i(\mathbf{y})\}$, respectively. Furthermore, let $\mathcal{S} \subseteq X$ be an arbitrary but fixed set. The *proper utility* $\mu(\mathbf{x}, \mathcal{S})$ of a point $\mathbf{x} \in \mathcal{S}$ is defined by

$$\mu(\mathbf{x}, \mathcal{S}) := \sup_{\mathbf{y} \in \mathcal{S}} \max_{i \in I_>(\mathbf{x},\mathbf{y})} \min_{j \in I_<(\mathbf{x},\mathbf{y})} \frac{f_i(\mathbf{x}) - f_i(\mathbf{y})}{f_j(\mathbf{y}) - f_j(\mathbf{x})}. \quad (2)$$

The proper knee $\mathbf{x}_{PK}$ is the minimizer of $\mu(\mathbf{x}, \mathcal{S})$. It can be related to the weighted sum as follows.

THEOREM 2. *Let $m = 2$ and an optimization problem be given. Then, the proper knee corresponds to the point that minimizes the sum of both objectives, i.e.,*

$$\arg \inf_{\mathbf{x} \in X_p} \mu(\mathbf{x}, X_p) = \arg \inf_{\mathbf{x} \in X} (f_1(\mathbf{x}) + f_2(\mathbf{x})).$$

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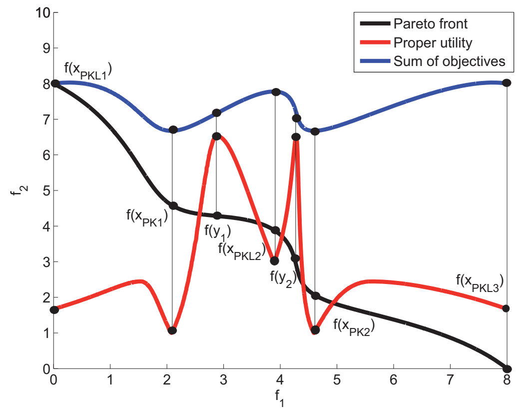

Figure 1: Fitness landscape according to proper utility values and the overall sum of objectives. While the sum of objectives utility correctly identifies $f(\mathbf{x}_{PK1})$ and $f(\mathbf{x}_{PK2})$ as global and $f(\mathbf{x}_{PKL1})$ and $f(\mathbf{x}_{PKL3})$ as local proper knees, it entirely misses $f(\mathbf{x}_{PKL2})$. The point $f(\mathbf{x}_{PKL2})$ is falsely identified as local maximum and the actual maxima $f(\mathbf{y}_1)$ and $f(\mathbf{y}_2)$ correspond to the inflection points of the sum of objectives curve.

While Theorem 2 allows to find the proper knee in an easy and convenient way for two objectives, it provides no conclusion to how the utility landscape of a Pareto front is actually shaped. Minimizing the sum of both objectives yields a completely different result as depicted in Figure 1.

4. KNEE FINDING ALGORITHMS

In order to find the knee, one could use the knee definition to induce a total order among the elements in the objective space. We do this for the weighted sum and the proper knee and investigate the theoretical and algorithmic implications.

We use the following dominations in NSGA-II to induce a complete ordering.

Definition 1 (w-domination and U-domination [6]). *A solution* $\mathbf{u} \in X$ w-dominates *a solution* $\mathbf{v} \in X$ *denoted as* $\mathbf{u} \succ_w \mathbf{v}$ *if* $\sum_{i=1}^m \mathbf{u} \leq \sum_{i=1}^m \mathbf{v}$*, A solution* $\mathbf{u} \in X$ U-dominates *a solution* $\mathbf{v} \in X$ *denoted as* $\mathbf{u} \succ_U \mathbf{v}$ *if either* $\mathbf{u}$ *Pareto-dominates* $\mathbf{v}$*, or if* $\mathbf{u}$ *and* $\mathbf{v}$ *are nondominated and additionally* $\mu(\mathbf{u}, \{\mathbf{u}, \mathbf{v}\}) < \mu(\mathbf{v}, \{\mathbf{u}, \mathbf{v}\})$ *holds.*

We used the w-domination and the U-domination in NSGA-II (instead of Pareto domination) and computed the number of function evaluation required to approximate the knee to a certain accuracy. The fitness landscape plays here an important role, although the proper knee is the same as the weighted sum solution in the case of two objectives and if equal weights are used (from Theorem 2). The statistical results (51 runs for each problem) are summarized in Tables 1 and 2. The values in bold show the better of the two dominations. The proper utility and the sum of objective functions of ZDT1 and ZDT2 are unimodal with just one (local and global) proper knee. In such a case applying a weighted sum method works better than the trade-off based approach of U-domination. The weighted sum also is also a clear winner if a very good approximation ($\epsilon = 1e-4$) needs to be found. However, for knee test problems, which exhibit many local and global minima (and inflexion points, see Figure 1), U-domination works best, especially if crude approximation of the knee is to be found. This can be explained as follows. In problems with multiple KKT points, the weighted sum has more the chance of getting stuck. However, at the end if the weighted sum is closed to the basin of attraction of global optima, it can converge quickly. For difficult problem, it might be useful to start with a trade-off based domination and then later switch to a weighted sum based domination.

	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
DEB2DK(k=1)	4300	7700	12700	25100	**38900**
DEB2DK(k=3)	4300	**7600**	**11900**	**20200**	**52600**
DO2DK(k=2,s=1)	3300	**6700**	11100	**22100**	**63500**
DO2DK(k=4,s=1)	3100	6600	10600	**20400**	**69500**
ZDT1	**900**	**5100**	**9200**	**16300**	**35600**
ZDT2	**1600**	**5300**	**8600**	**12100**	**15600**

Table 1: Median number of function evaluations until the distance between the best found equal weighted sum and the exact proper knee falls below a threshold value ϵ.

	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
DEB2DK(k=1)	**4200**	**7500**	**12500**	**21500**	41100
DEB2DK(k=3)	**4200**	**7600**	12100	23200	96300
DO2DK(k=2,s=1)	**3200**	**6700**	**10600**	23500	82200
DO2DK(k=4,s=1)	**3000**	**6500**	**10400**	20700	78600
ZDT1	1000	5200	8700	17900	33300
ZDT2	**1600**	5400	8700	12200	**15600**

Table 2: Median number of function evaluations until the distance between the best found knee and the exact proper knee falls below a threshold value ϵ.

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