A model of anytime algorithm performance for biobjective optimization problems

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Abstract. Anytime algorithms allow a practitioner to trade-off runtime for solution quality. This is of particular interest in multiobjective optimization since it might be infeasible to identify the Pareto set in a reasonable amount of time. We present a theoretical model to characterize the trade-off between solution quality, in terms of relative hypervolume, and runtime for exact anytime algorithms for biobjective optimization problems. Our model works under some basic assumptions, such as, Pareto optimal solutions are collected sequentially and the Pareto front can be well approximated by a quadrant of a particular superellipse. We validate our model against an anytime algorithm based on the ϵ-constraint approach for the biobjective unconstrained knapsack problem.

INTRODUCTION

In a multiobjective combinatorial optimization problem, there is usually not a single solution which is optimal under the notion of Pareto optimality, but rather a set, the so-called Pareto set, that represents the trade-offs between the conflicting objectives [1]. In this work, we consider biobjective optimization problems with two objective functions

$$\max_{x \in X} f(x) = \max_{x \in X} (f_1(x), f_2(x)) \tag{1}$$

where X denotes the set of feasible solutions and "max" is considered under the notion of Pareto optimality. The image of X in the objective space is denoted by $Y = \{f(x) \mid x \in X\}$. For two solutions $x, x' \in X$ we introduce the following dominance relation: $f(x') < f(x)$, that is $f(x)$ *dominates* $f(x')$, iff $f_i(x') \leq f_i(x),\ i \in \{1, 2\}$ and $f(x') \neq f(x)$. A solution $x \in X$ is said to be *Pareto optimal* if no other solution $x' \in X$ exists such that $f(x) < f(x')$. Lastly, the set of all *Pareto optimal* solutions is called the *Pareto set*, and its image in the objective space is called the *Pareto front*.

Due to the possible intractability of the Pareto set [1], it might be infeasible to identify all solutions in a reasonable amount of time. As a result, it can be more relevant to seek a representative subset of the Pareto set that satisfies some interesting properties, such as, cardinality or solution quality guarantees [2]. Anytime algorithms [3] are an appealing concept for multiobjective optimization since they should, in principle, find improving representative subsets (or approximations which may contain non-optimal solutions) of the Pareto set at any time of the search process. An example of such an anytime approach is the ϵ-constraint technique [1] which collects Pareto optimal solutions by solving a sequence of constrained single-objective problems. In order to assess the performance of anytime algorithms, there is the need to relate solution quality, expressed as a subset of the Pareto set, with the time taken to achieve it. The trade-off between solution quality and runtime is called *anytime behavior*.

Several *quality indicators* have been proposed to measure the quality of a Pareto set approximation as a scalar value [4]. A commonly used indicator is the hypervolume [5], which corresponds to the measure of the multidimensional area dominated by a set of points $S \subseteq Y$, bounded by a reference point $r \in \mathbb{R}^2$, that is

$$H(S) = \lambda\left(\left\{q \in \mathbb{R}^2 \mid \exists\, s \in S : r \leq q \leq s\right\}\right) \tag{2}$$

where λ denotes the Lebesgue measure. For this work, we introduce the notion of hypervolume contribution, which is the hypervolume contribution of a point $t \in Y$ with respect to a set of of points $S \subseteq Y$ and is given by $H(t, S) = H(S \cup \{t\}) - H(S)$. Interestingly, the hypervolume increases monotonically with more Pareto optimal solutions and is maximal when the Pareto set is found [4].

The study of the anytime behavior for multiobjective optimization has recently gotten some attention. In [6], a hybrid evolution strategy for biobjective optimization is shown to provide a good anytime behavior, measured in terms of solution quality (hypervolume) achieved after different time budgets in a certain range. In [7], the anytime behavior of a local search method, measured in terms of hypervolume for the trade-off between solution quality and runtime, is analyzed. Algorithm components from the original approach are improved and refined in order to achieve a better anytime behavior. However, up to our knowledge, most studies on anytime multiobjective optimization have been empirical and focused on heuristics which provide no guarantee on the optimality of the solutions.

In this work, we are particularly interested in characterizing the performance of anytime exact algorithms that maximize the hypervolume by sequentially collecting Pareto optimal solutions. We study its performance in terms of the trade-off between runtime and relative hypervolume, that is, the current hypervolume relative to the maximal hypervolume of the Pareto front. In particular, we propose a theoretical model that estimates this trade-off for biobjective optimization under the assumption that the "shape" of the Pareto front can be approximated by a quadrant of a particular superellipse. The model works by collecting minimal information about the Pareto front, which allows us to approximate it with a piecewise linear curve. From this curve, we assume an oracle that returns, at each call, a point that maximizes the hypervolume contribution.

We show that the relation between the number of calls of this oracle (runtime) and the relative hypervolume value achieved can be expressed by a simple piecewise linear function that depends on a "curvature" parameter of the piecewise curve. We validate our model against the performance of an "anytime" version of the ϵ-constraint technique for the unconstrained biobjective knapsack problem.

A HYPERVOLUME/RUNTIME THEORETICAL MODEL

In this section we present a theoretical model to estimate the trade-off between solution quality and runtime for a biobjective optimization problem. We assume an oracle that returns, at each call, a point in the objective space that maximizes the hypervolume contribution. Note that, since the hypervolume is a monotone submodular function [8], this oracle returns, after i calls, an $(1 - 1/e)$-approximation to the optimal hypervolume value for i points [9]. For clarity of exposition we split our model into two parts. First, we define a piecewise linear approximation of the Pareto front under some assumptions, that is, we assume that the objective values of the lexicographic optimal solutions are known and that the Pareto front can be well approximated by a certain family of curves. Then, given this piecewise linear approximation, we are able to derive equations that estimate the relative hypervolume after i calls to the oracle.

Estimating the Pareto front as a piecewise linear function We assume that the Pareto front, scaled down to the unit square $[0, 1]^2$, can be approximated by the positive quadrant of a particular superellipse centered in the origin with both semi-diameters of length one, which is given by the following parametric equation (in Cartesian coordinates)

$$y_1{}^d + y_2{}^d = 1 \tag{3}$$

where $d > 0$ is a parameter that controls the curvature of this particular superellipse and $y_1, y_2 \in [0, 1]$. Although it is not expected that the Pareto front is a convex curve, our empirical findings suggest that this gives a good approximation in practice for many problems with linear sum objective functions. Such superspheres have been studied in [10].

We consider a piecewise linear approximation to this curve by defining a point (p, p), such that $p = 2^{-\frac{1}{d}}$, and the corresponding piecewise linear function in Equation 4. The maximal hypervolume for this approximation with reference point $r = (0, 0)$ is given by p.

$$g(y_1) = \begin{cases} \frac{p-1}{p} y_1 + 1 & , 0 \leq y_1 \leq p \\ \frac{p}{p-1} y_1 + \frac{p}{1-p} & , p < y_1 \leq 1 \end{cases} \tag{4}$$

An oracle for the largest hypervolume contribution Let us define an oracle that collects a sequence of points from the piecewise linear approximation, each of which providing the largest hypervolume contribution. Let C_i denote the hypervolume contribution of the ith point returned by the oracle.

Assuming $p \geq 0.5$ and a fixed hypervolume reference point $r = (0, 0)$, the first point returned by the oracle is (p, p), which can be found by maximizing $y_1 \cdot g(y_1)$. Thus, the initial hypervolume contribution is $C_1 = p^2$. The following point returned by the oracle is calculated by considering the dominated regions that remain uncovered, which correspond to two identical right triangles with catheti of size $1 - p$ and p. The point providing the largest hypervolume contribution for a right triangle with reference point on its right angle, is given by the intersection of the perpendicular lines that split the catheti in half. Thus, the following two largest hypervolume contributions will be equal to half the area of the right triangles and given by $C_2 = C_3 = ((1 - p) \cdot p)/4$. Furthermore, after excluding the regions dominated by these points, the remaining uncovered dominated regions are given by four right triangles, each of which has catheti with half the length of the original right triangles and, consequently, a quarter of the area. Since C_1 is known and, after that, the number of equivalent right triangles grows by powers of two and their area decreases by a quarter each time, a general equation for C_i at the ith call of the oracle can be obtained as follows

$$C_i = \begin{cases} p^2 & i = 1 \\ \dfrac{(1 - p) \cdot p}{4^{\lfloor \log_2 i \rfloor}} & i \geq 2 \end{cases} \tag{5}$$

Let $D_i = C_1 + C_2 + \ldots + C_i$ be the hypervolume of the set of points collected up to the ith call of the oracle. Then, the relative hypervolume up to the ith call is given by D_i/p. Note that, the (relative) hypervolume has a logarithmic rate of convergence. For the case of $p < 0.5$, Equation 5 does not hold. However, it is possible to compute the hypervolume contributions by taking advantage of the remaining dominated areas, which are either triangles or the union of two triangles. Nonetheless, a more detailed study for $p < 0.5$ will be considered in a further extension of this work.

EMPIRICAL STUDY

In order to validate our model and its relevance for practical anytime biobjective optimization algorithms, we compare the relative hypervolume obtained from our theoretical model with a technique that at each step finds a Pareto optimal solution. More particularly, we consider the ϵ-constraint [1] that solves a sequence of constrained single-objective problems by transforming one of the objectives into a constraint. At each step, the right hand side of the constraint is varied over the range of values of the objective function. In our case, for the first iteration of the ϵ-constraint, we set the value of the right hand side of the constraint to p. Then, our approach bisects the intervals $[0, p]$ and $[p, 1]$ which provides a new right hand side p_1 and p_2, respectively. This procedure is repeated for each point found until some termination criterion is met. We expect that, by setting the right hand side values of the constraint with this bisection, the ϵ-constraint technique will approximate the behavior of our oracle.

We consider the unconstrained knapsack problem. Formally, given a set of items J, where each item $j = 1, \ldots, |J|$ has a profit p_j and weight w_j, the unconstrained knapsack problem is defined as

$$\max \left(f_1(x) = \sum_{j=1}^{|J|} p_j x_j,\ f_2(x) = -\sum_{j=1}^{|J|} w_j x_j \right) \tag{6}$$

where x_j denotes a binary variable that indicates whether or not item j has been chosen for the knapsack. In order to be consistent with the theoretical model, we scale the objective functions into the range $[0, 1]$.

In order to determine the value of parameter p required by our model we average the objective values of a Pareto front point found with a weighted-sum method. We consider the scalarized formulation $\max w f_1(x) + (1 - w) f_2(x)$ for $w = 0.5$. Let x' be the optimal solution to the weighted sum and y_1 and y_2 be the normalized objective values of x' for f_1 and f_2 respectively, then we define $p = (y_1 + y_2)/2$.

We validated our model against the ϵ-constraint approach using a linear programming solver (GNU Linear Programming Kit MILP Solver) on multiple problem instances with a variable number of items and correlation between the items. Figure 1 shows the evolution of relative hypervolume for the first 128 steps of the ϵ-constraint algorithm (solid line) and calls to the oracle (dashed line), for three selected instances with $|J| = 100$ and varying correlation. The experimental results indicate that our simple model approximates quite well the performance of the ϵ-constraint approach as the runtime increases. The largest differences are found only in the first steps since the maximal hypervolume of the linear approximation (given by p) is smaller than that of the complete Pareto front (calculated using an exact approach [11]) for the considered instances. This difference vanishes with increasing correlation between the objectives since our model can better approximate the Pareto front in those cases (p becomes closer to 0.5). Moreover, our experiments revealed that different problem sizes do not seem to affect the results.

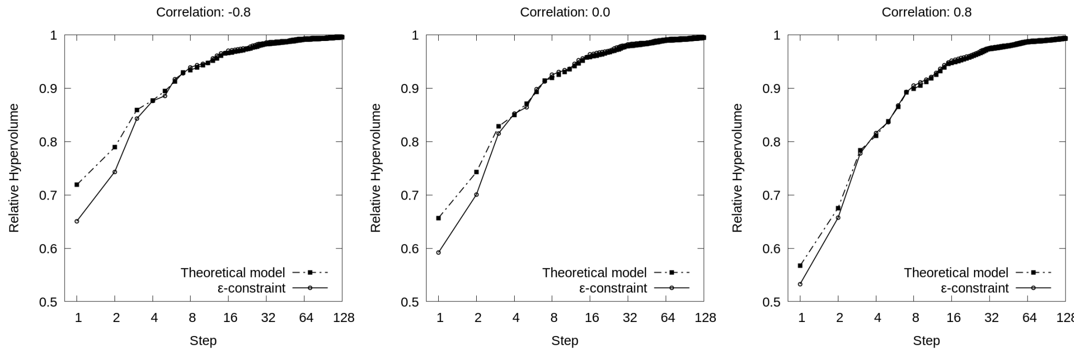

FIGURE 1. Comparison of the relative hypervolume between the theoretical model and the ϵ-constraint algorithm

CONCLUSION

In this work, we presented a simple theoretical model to characterize the trade-off between runtime and hypervolume in the context of anytime algorithms for biobjective optimization problems. The experimental results indicate that the model approximates quite well the performance of an anytime variant of the ϵ-constraint algorithm for the unconstrained knapsack problem. Further research consists of developing a more fine-grained model, for instance, considering more initial points in order to provide a better approximation for the initial steps. Moreover, although the case of $p < 0.5$ can be modeled algorithmically, we aim to extend our analytical model for this case. Note that the runtime to find each Pareto optimal solution with the ϵ-constraint approach did not change considerably. However, this may not be true for other algorithmic paradigms, for which a larger variance is expected. For those cases, our model should consider a different measure of runtime. Finally, an interesting application of our findings is on algorithm survival analysis [12]. Based on our model it is possible to understand whether an exact approach is taking too much time to find the next Pareto optimal solution, which may justify a restart or a switch to a different search strategy.

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