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Direct zigzag search for discrete multi-objective optimization

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ABSTRACT

Multiple objective optimization (MOO) models and solution methods are commonly used for multi-criteria decision making in real-life engineering and management applications. Much research has been conducted for continuous MOO problems, but MOO problems with discrete or mixed integer variables and black-box objective functions arise frequently in practice. For example, in energy industry, optimal development problems of oil gas fields, shale gas hydraulic fracturing, and carbon dioxide geologic storage and enhanced oil recovery, may consider integer variables (number of wells, well drilling blocks), continuous variables (e.g. bottom hole pressures, production rates), and the field performance is typically evaluated by black-box reservoir simulation. These discrete or mixed integer MOO (DMOO) problems with black-box objective functions are more challenging and require new MOO solution techniques. We develop a direct zigzag (DZZ) search method by effectively integrating gradient-free direct search and zigzag search for such DMOO problems. Based on three numerical example problems including a mixed integer MOO problem associated with the optimal development of a carbon dioxide capture and storage (CCS) project, DZZ is demonstrated to be computationally efficient. The numerical results also suggest that DZZ significantly outperforms NSGA-II, a widely used genetic algorithms (GA) method.

1. Introduction

Decision making problems with multiple criteria arise in various fields of engineering and sciences [1–6]. It is often not possible that a decision (e.g. an inventory control policy or a production system design plan) simultaneously optimizes all the considered criteria. There are, instead, a set of alternatives that trade off the decision criteria. Multi-criteria decision making problems can typically be analyzed with multi-objective optimization (MOO) models. Researchers and practitioners in mathematics, operations research, engineering, and management sciences, have conducted a tremendous amount of work to develop theories, methodologies, and applications of MOO. Many real-world MOO problems include integer ordered or discrete decision variables. Such discrete multi-objective optimization (DMOO) is more challenging due to the discontinuity of objective functions and the discreteness of optimal solution set. In this work, DMOO problems with discrete decision variables and black-box objective functions are particularly of interest.

Most of existing research in multi-criteria decision making is for deterministic and continuous MOO problems with closed-form objective functions [7–14]. Current methods for continuous MOO problems fall into two broad categories: (i) population-based stochastic search methods and (ii) iterative pointwise solution search methods. In category (i), many population-based methods for MOO problems are variants of evolutionary algorithms, e.g. genetic algorithms (GA) [15–20] and particle swarm optimization (PSO) [21,22]. Evolutionary algorithms are widely used particularly as comparison methods because they are general and relatively easy to implement. The slow convergence, if they have however, makes them impractical for many real-world MOO problems, where the objective function evaluations may entail intense computing. Much MOO research has been in development of the category (ii) of iterative pointwise solution search algorithms that typically solve a sequence of parameterized single-objective optimization subproblems for a sequence of Pareto optimal solutions [23–25], including the popular weighted sum method [13] and the normal boundary intersection method [11]. Continuation based methods [26,27,14,28–31] that are capable of tracing a Pareto front (characterized by a continuous manifold) have been developed recently. Some other important development for continuous MOO of category (ii) includes zigzag search [32] and other local search based algorithms [33,34]. Refer to [35,36,1] and recent books [9,12,37] for detailed discussions of existing methods, analysis, and applications of continuous MOO.

DMOO problems commonly exist in real-life engineering and management projects, but efficient algorithms for discrete and black-box MOO problems are still missing. To fill this important gap and develop practical solution methods, we propose a new DMOO method based on a direct zigzag (DZZ) search approach. DZZ method searches Pareto optimal solutions along a zigzag path close to the Pareto front. The local zigzag path is identified based

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on a direct search approach (e.g., Hooke Jeeves method [38] or pattern search [39]) in which the search procedure only compares function values without computing the gradients of objective functions. Thus, DZZ is general and can be applied for black-box DMOO problems, where the objective functions are evaluated through numerical or simulation processes. DZZ also guarantees the local Pareto optimality (discussed in Section 3.4), due to the neighborhood search employed within the direct search procedure. We demonstrate the DZZ efficiency using three DMOO example problems including an optimal development case of carbon subsurface sequestration. The optimization performance of DZZ is compared to that of a non-dominated sorting genetic algorithm (NSGA-II) [40], one state-of-the-art method in the family of Genetic Algorithms. The promising optimization results of DZZ suggest that DZZ outperforms NSGA-II in terms of optimization efficiency and solution quality.

The rest part of the paper is organized as follows. Section 2 provides a formal statement of DMOO problems and introduces some relevant concepts of MOO. Section 3 discusses the details of the DZZ search method and presents one algorithmic implementation of DZZ, specifically for bi-objective optimization problems. In Section 4, we test the proposed DZZ algorithm on three example problems including two taken from the recent literature and one example case in the carbon geologic sequestration project. Conclusions and future research are discussed in the last section.

2. Problem statement

General mixed integer MOO problems with both integer-valued and continuous variables are formulated as follows.

(P) min $f(x),\ x \in \{\mathbb{Z}^{d_1} \times \mathbb{R}^{d_2}\}$,
Subject to $h_i(x) \le 0,\ i = 1, 2, \ldots, l.$

Let $\mathbb{X}$ denote the feasible region in (P) and $d = d_1 + d_2$. The feasible region $\mathbb{X}$ is a set in the d-dimensional mixed integer space that can be in general specified by l inequality constraints $h_i(x) \le 0, i = 1, 2, \ldots, l$; for unconstrained MOO problems, $l=0$. These constraint functions are assumed to be deterministic with closed functional forms. Within (P) the objective function $f : \mathbb{Z}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}^k$ is defined by an analytic function or implicitly defined by computer simulation processes. In the context of optimal development of the carbon geological sequestration project, for example, a bi-objective f could be the total quantity of carbon dioxide injected into the storage field and the amount of mobile carbon that has risk of leakage after a long storage time, say 1000 years. The goal of (P) is to seek local Pareto optimal solutions of the objective function f on $\mathbb{X}$. The definition of Pareto optimality is provided below.

Definition 1. For solutions $x, y \in \mathbb{X}$, x is said to weakly dominate y, denoted as $x \succcurlyeq y$, if $f_i(x) \le f_i(y)$ for $i = 1, 2, \ldots, k$. A solution $x \in \mathbb{X}$ strictly dominates or simply dominates $y \in \mathbb{X}$, denoted as $x \succ y$, if $x \succcurlyeq y$ and there exists at least one $i \in \{1, 2, \ldots, k\}$ so that $f_i(x) < f_i(y)$.

Definition 2. A solution $x \in \mathbb{X}$ is globally Pareto optimal or simply Pareto optimal if there is no $y \in \mathbb{X}$ such that $y \succ x$. A solution $x \in \mathbb{X}$ is said to be locally Pareto optimal for a neighborhood $N_\delta(x)$ associated with x if no $y \in N_\delta(x) \cap \mathbb{X}$ satisfying $y \succ x$. The function values $f(X^*)$ for (local) Pareto solutions X^* displayed in the objective space form the (local) Pareto front. A useful definition of N_δ is discussed below.

Definition 3. Let $x = (x_1, x_2), x_1 \in \mathbb{Z}^{d_1}, x_2 \in \mathbb{R}^{d_2}$ be a feasible solution in $\mathbb{X}$. The δ-neighborhood $N_\delta(x)$ of x includes feasible points $y = (y_1, y_2) \in \mathbb{X}$ so that $\|x - y\| \le 1$ and $\|x_2 - y_2\| \le \delta$, where $y_1 \in \mathbb{Z}^{d_1}$ and $y_2 \in \mathbb{R}^{d_2}$.

For general mixed integer MOO problems, i.e. $d_2 \ne 0$ in (P), Definition 3 defines a neighborhood at x that includes a number of ($2d_1$ or fewer) separate points that are 1 unit distance away from x and a set of points within a hypercube centered at x of dimension δ in $\mathbb{R}^{d_2}$. In numerical algorithm design, to verify a local Pareto optimum with the neighborhood N_δ is computationally expensive and error prone. Thus we consider δ-approximate Pareto optimality based on a discrete (finite) neighborhood as stated in Definition 4.

Definition 4. Given a $\delta > 0$, a feasible solution $x^* \in \mathbb{X}$ is a δ-approximate local Pareto minimum to (P) if $x^* \succcurlyeq y$ for any $y \in S_\delta(x^*)$, where $S_\delta(x^*) = \{y = (y_1, y_2) \in \mathbb{X} : \delta \le \|x^* - y\| \le 1, \|x_2^* - y_2\| \le \delta\}$ consists of $2d$ or fewer feasible points near x^*.

We develop a new DMOO method, termed DZZ, to quickly identify a set of well-distributed *approximate* local Pareto optima of (P) based on the above δ-approximate optimum definition. If $d_2 \ne 0$ in (P), we consider a small enough $\delta > 0$ so that DZZ returns a set of δ-approximate local Pareto optimal solutions to (P). If $d_2 = 0$, then (P) is a DMOO problem with integer decision variables. In this case, a neighborhood definition with $\delta = 1$ will be $N_1(x) = \{y \in \mathbb{X} : \|x - y\| = 1\}$. For general DMOO problems with the feasible set $\mathbb{X} \subset \mathbb{R}^d$ containing a set of (finite or countably infinite) discrete points, we may define a generic neighborhood structure $N(x)$ that contains $2d$ or fewer feasible points closest to x coordinate-wise. Specifically,

$$N(x) = \begin{cases} (y_1, \ldots, y_i, \ldots, y_d) \in \mathbb{X} : y_i = \arg\min_{y_i} (x_i - y_i) & \text{if } x_i \ge y_i, \forall j \ne i, x_j = y_j, i = 1, 2, \ldots, d \\ (y_1, \ldots, y_i, \ldots, y_d) \in \mathbb{X} : y_i = \arg\min_{y_i} (y_i - x_i) & \text{if } x_i < y_i, \forall j \ne i, x_j = y_j, i = 1, 2, \ldots, d, \end{cases}$$

where x_i and y_i are the ith coordinates of x and y respectively. An alternative neighborhood for DMOO is based on Delaunay

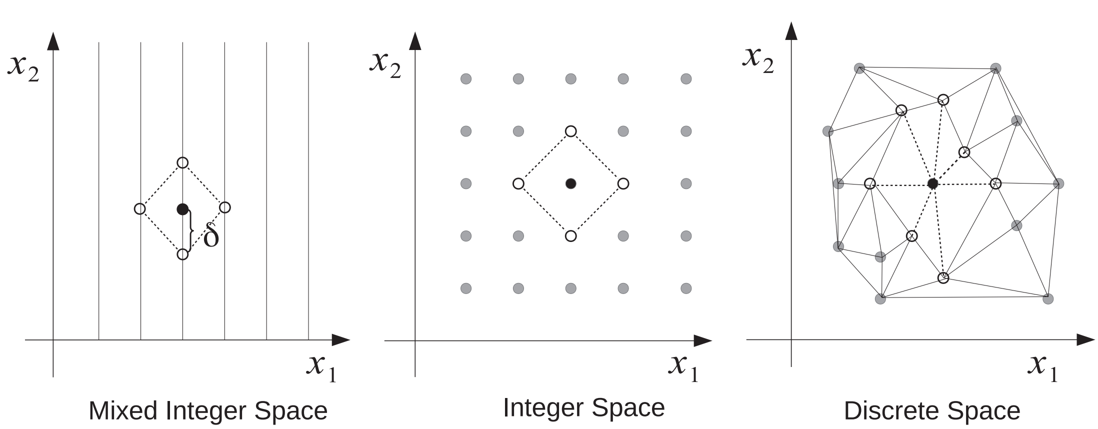

Fig. 1. Example neighborhood structures for mixed integer, 2-dimensional integer, and discrete solution spaces.