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Algorithms for Finding Maximum Diversity of Design Variables in Multi-Objective Optimization

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Abstract

This paper considers the problem of finding architectures with sufficient multi-objective Pareto optimality and maximum diversity of their design-variable values. This problem has been exclusively addressed to date by Evolutionary Algorithms, which are known to be powerful, and yet, the optimality of their solutions cannot be guaranteed. This paper defines two somewhat dual Maximal Design Diversity (MDD) problems, namely, (1) Primal p-MDD: maximizing a design-variable diversity metric between p architectures given a margin for compromising Pareto optimality, and (2) Dual p-MDD: minimizing the compromise of Pareto optimality of p architectures given a lower bound for design-variable diversity. Greedy algorithms for computing both Primal and Dual p-MDD are presented. For the Primal p-MDD the proposed greedy algorithm is proven to be a 2-approximation of the optimal algorithm and an upper bound for the optimality violation is computed, with respect to the efficient frontier in the objective space. For the Dual p-MDD the optimality violation of the proposed greedy algorithm is proven to be at least as good as that of the optimal algorithm when the lower bound on the distance between the solutions in the design-variable space is doubled. Finally, a real-world mixed-integer non-linear programming model with two objectives, dozens of variables and hundreds of constraints is considered as the main use case, taken from the domain of aircraft-engine design. The results validate the fidelity of the algorithm.

Keywords: Design variables diversity maximization, architecture diversity maximization, algorithms, mathematical programming;

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1. Introduction

Diversity in the design-variable space of a multi-objective problem is of much interest as a vehicle to find the rich collection of product and process architectures that employ different mechanisms to achieve the same goal. Many of the most important considerations that determine the business efficacy of an architecture are difficult or impractical to model in an objective function, e.g., strategic alignment, competitive positioning, intellectual property, supplier capabilities, manufacturability, market desirability. Therefore, it is competitively advantageous to be able to generate a comprehensive list of the most diverse architectures spanning the design space, all mapped onto the proximity of the efficient frontier, and evaluate them both quantitatively and qualitatively to find those with the greatest real value.

Existing methods to find near-optimal solutions with the greatest diversity of design variable values are exclusively based upon Evolutionary Algorithms (EAs), where the coined terminology is *decision-space diversity*. Within this rich domain it is worth noting studies by Ulrich et al. [6, 7], Deb's Omni-Optimizer [2], and the work of Shir et al. [4] on a niching approach to this problem. EAs are powerful bio-inspired population-based optimizers that primarily excel in black-box scenarios, where the objective function cannot be analytically formulated (e.g., in simulation-based optimization or experimental optimization). On the other hand, upon consideration of analytical optimization problems that may be treated by mathematical solvers, EAs may not be the best tool for this problem, due to their incomplete consideration of the space, their consequent lack of an optimality guarantee, and their computational overhead, due to the large number of iterations and the population sizes typically employed. Thus, an algorithm that would guarantee both proximity to the efficient frontier as well as high design-space diversity, and that would require only a few iterations to accomplish that, is of great interest.

The current study introduces two Maximal Design Diversity (MDD) problems, which may be considered to be dual to some extent. The first maximizes a design-variable diversity metric, while considering a given bound for compromising the Pareto optimality. The other minimizes the degree of compromise of the Pareto optimality, subject to a lower bound for design-variable diversity. Algorithms for computing both problems are then described and theoretical results are presented. A real-world application, a Mixed-Integer Non-Linear Programming (MINLP) model use case, which is taken from the field of aircraft engine design, is then considered. This work concludes with a discussion.

2. Problem Formulation

In this section two somewhat *dual* problems are defined: (1) maximizing the design-variable diversity metric, given a bound on the compromise of Pareto optimality; (2) minimizing the compromise of Pareto optimality, given the required degree of design-variable diversity. The notation follows Masin and Bukchin [3].

Assumption 1 Without *loss of generality, let us define the following multi-objective vector minimization problem:* Minimize $y = \{f^{(1)}(x), f^{(2)}(x), \dots, f^{(K)}(x)\}$ subject to $x \in X$, *where* $X \subset R^n$ *is a set of feasible solutions,* $Y \subset R^K$ *is its image in the objective space, and* $f: X \to Y$ *is an objective function that projects* X *to* Y.

If $x \in X$, then $y = f(x) \in Y$ and the value of the i^{th} objective of solution x is $y^{(i)} = f^{(i)}(x)$. For $x_1, x_2 \in X, y_1 = f(x_1), y_2 = f(x_2) \in Y$, let $y_1 = y_2$ and $y_1 \leq y_2$ if $y_1^{(i)} = y_2^{(i)}$ and $y_1^{(i)} \leq y_2^{(i)}$ for all i, respectively. Two solutions $x_1, x_2 \in X, y_1 = f(x_1), y_2 = f(x_2) \in Y$ are equivalent if $y_1 = y_2$. We write $y_1 < y_2$ if $y_1^{(i)} \leq y_2^{(i)}$ for all i and $y_1^{(i)} < y_2^{(i)}$ for some i. In this case, we would say that y_2 is dominated by y_1, or y_1 dominates y_2.

Assumption 2 *We* assume *that the set* X *is compact and each of the objective functions* f *is continuous.*

Let X_{Par} denote the complete set of Pareto optimal solutions in X, i.e., solution $x \in X_{\text{Par}}$ if and only if there is no $x_1 \in X$ such that $f(x_1) < f(x)$. If solution x is Pareto optimal, then we call $y = f(x)$ efficient.

The complete set of efficient points in the objective space, Y_{eff} , is called the efficient frontier. As previously discussed, the set X_{Par} may contain equivalent solutions, or in other words, a single efficient point $y \in Y_{\text{eff}}$ may be mapped onto multiple equivalent pre-images in X_{Par}.

Let $d_X(\cdot,\cdot)$ be a metric on X. Recall that for a metric a triangle inequality is satisfied, i.e., for all $x_1, x_2, x_3 \in X, d_X(x_1, x_3) \leq d_X(x_1, x_2) + d_X(x_2, x_3)$. Also, for any subset $V \subseteq X$ and any point $x \in X$, $d_X(x, V) = \min\{d_X(x, v) | v \in V\}$. We denote $d_X(x, V)$ by $d_V(x)$. Furthermore, let $d_E(y)$ be a function representing a measure for distance in the objective space. In this paper we use $d_E(y) = \min_{e \in E} \max_{i=1,\dots,K} y^{(i)}/y_e^{(i)} - 1$, where $E \subset Y$, but other functions could be defined as well. Let δ_E be a prescribed constant defining the maximally accepted distance away from a set E with respect to $d_E(y)$. Let δ_V be a prescribed constant defining the minimally accepted distance from a set V. We are now in a position to define two optimization problems .

Definition 1 *A **Primal MDD** problem is:* $Maximize\ d_V(x)$, subject to $x \in X, y = f(x)$, $d_E(y) \leq \delta_E$.
Definition 2 *A **Dual MDD** problem is:* $Minimize\ d_E(y)$, subject to $x \in X, y = f(x)$, $d_V(x) \geq \delta_V$**.**

In the Primal MDD, the diversity in the design-variable space is enhanced by compromising the Pareto optimality by δ_E within the objective space. The diversity is expected to get higher as larger δ_E values are considered. On the other hand, in the Dual MDD the aim is to locate the closest solution in the objective space that is far enough with respect to the set V, at least δ_V, in the design-variable space. Upon searching for more than a single solution, Primal and Dual MDDs could be extended to the following Primal p-MDD and Dual p-MDD problems. Let $S_p = \{V \subseteq X: d_E(f(x)) \leq \delta_E, \forall\ x \in V\}$ be a set of feasible solutions for Primal p-MDD problem. Let $S_d = \{V \subseteq X: d_X(x, V \backslash \{x\}) \geq \delta_V, \forall\ x \in V\}$ be a set of feasible solutions for Dual p-MDD problem.

Definition 3 *A **Primal p-MDD** problem is a problem of finding the set* $V = \{x_1, \cdots, x_p\} \in S_p$, *such that* $min_{1 \leq i \neq j \leq p}\{d_X(x_i, x_j)\}$ *is maximized.*
Definition 4 *A **Dual p-MDD*** problem *is a problem of finding the set* $V = \{x_1, \cdots, x_p\} \in S_d$, *such that* $max_{1 \leq i \leq p} d_E(f(x_i))$ *is minimized.*

3. Algorithms for Finding Maximum Diversity of Design Variables

3.1 Primal Maximum Design Diversity Approximation Algorithm

The idea behind this algorithm, shown in the left column of Fig. 1, is to start from a partial efficient frontier, E, as well as an initial solution in the design-variable space. Then, at each iteration, the algorithm adds the farthest solution in the design-variable space to the existing subset of feasible solutions, as summarized in Algorithm 3.1. In Step 1, the design-variable and objective spaces are initialized. The values for the maximally allowed distance in the objective space and the maximal number of iterations are set. In Step 2 a Primal MDD optimization problem is solved and in Step 3 the current set of design variables V is augmented by x^* when x^* is an optimal solution. The procedure in Step 2 is repeated until either the maximal number of iterations is reached or no feasible solution exists. In Step 4, the design-variable set V is returned.

Theorem 1 *Let V be the set of* solutions *(points in the design variables space) generated by Algorithm 3.1. Then V is a* $2-approximation$ *solution of the Primal* $|V|$*-MDD problem.*

Proof: The idea of the proof is based on Tamir [5]. Let V^* be an optimal solution of Primal p-MDD problem with the optimal value of δ^*, i.e., $d_X(x_1, x_2) \geq \delta^*$ for all distinct $x_1, x_2 \in V^*$. In Step 2 of iteration j of Algorithm 3.1, for each $x \in V^*$ with $d_V(x) < \delta^*/2$ there is a solution $\tilde{x} \in V$ such that $d_X(\tilde{x}, x) < \delta^*/2$. Moreover, for each $\tilde{x} \in V$ there is at most one $x \in V^*$ such that $d_X(\tilde{x}, x) < \delta^*/2$. That follows from $d_X(x_1, x_2) \geq \delta^*$ for all distinct $x_1, x_2 \in V^*$ and the triangle inequality of metric $d_X(\cdot,\cdot)$. In each iteration j of Step 2 holds $|V| < |V^*|$, therefore there exists a feasible solution $x \in V^*$ with $d_V(x) \geq \delta^*/2$. Finally, Primal MDD optimization problem maximizes $d_V(x)$ and the proof follows. □

Let $\xi_E(U) = \max_{x \in U} d_E(f(x))$ be the optimality violation for any set $U \subseteq X$ with respect to E.

Theorem 2 *Let V be the set of solutions generated by Algorithm 3.1. Then, $\xi_E(V) \leq \delta_E$.*

Proof: From Primal MDD optimization problem constraints follows that each $x \in V$ satisfies $d_E(f(x)) \leq \delta_E$ and the proof follows. □

3.1 Primal Greedy Algorithm for Finding Maximum Diversity of Design Variables	**3.2 Dual Greedy Algorithm for Finding Maximum Diversity of Design Variables**
1. Initialize: (a) Find $V_1 = \{x_1\} \subseteq X_{Par}, E \subseteq E_{eff}$ (b) Set $V = V_1$, $\delta_E =$ (maximal distance in objective space), $j = 2$, $J =$(maximal number of iterations). **2. Solve** Primal MDD optimization problem. If there is a feasible solution then $y^* = f(x^*)$ is the optimal solution, else go to Step 4. **3. Set** $V_j = V_{j-1} \cup \{x^*\}$ and $V = V_j$, $j = j + 1$. If $j > J$, go to Step 4, otherwise go to Step 2. **4. Return** V.	**1. Initialize**: (a) Find $V_1 = \{x_1\} \subseteq X_{Par}, E \subseteq E_{eff}$ (b) Set $V = V_1, j = 2$, $J =$ (maximal number of iterations). **2. Solve** Dual MDD optimization problem. If there is a feasible solution then $y^* = f(x^*)$ is the optimal solution, else go to Step 4. **3. Set** $V_j = V_{j-1} \cup \{x^*\}$ and $V = V_j$, $j = j + 1$. If $j > J$, go to Step 4, otherwise go to Step 2. **4. Return** V.

Fig. 1. Algorithms for Primal and Dual p-MDD problems

3.2 Dual Maximum Design Diversity Approximation Algorithm

In this section we show how Algorithm 3.1 could be adjusted to the Dual p-MDD problem, where the compromise of Pareto optimality is minimized subject to the minimal distance in the design-variable space. A listing of the algorithm appears as Algorithm 3.2 in the right column of Fig. 1. In Step 1, the design variables and objective spaces are initialized. The maximal number of iterations is set. In Step 2 a Dual MDD optimization problem is solved and in Step 3 the existing set of design variables V is augmented by x^* when x^* is an optimal solution. The procedure in Step 2 is repeated until the maximal number of iterations is reached or no feasible solution exists. In Step 4, the design-variable set V is returned.

Let $V_J^{opt} = \{argmin_U \xi_E(U): |U| = J, \delta_V = \eta\}$. Let V be the set of solutions generated by Algorithm 3.2 when $\delta_V = \eta/2$ and the number of iterations is J.

Theorem 3 *Let V_J^{opt} and V be* the *optimal and greedy solution sets of the Dual J-MDD problem with $\delta_V = \eta$ and $\delta_V = \eta/2$, respectively. Then, the optimality violation of the greedy algorithm is at least as good as the optimal algorithm. Namely, $\xi_E(V) \leq \xi_E(V_J^{opt})$. Moreover $|V|$=J.*

Proof: The proof is similar to the proof of Theorem 1. Let V_J^{opt} be an optimal solution of Dual J-MDD problem with the optimal value of δ^*, i.e., $d_E(f(x)) \leq \delta^*$ for all $x \in V_J^{opt}$, and $\delta_V = \eta$, i.e., $d_X(x_1, x_2) \geq \eta$ for all distinct $x_1, x_2 \in V^*$. In Step 2 of iteration j of Algorithm 3.2, for each $x \in V_J^{opt}$ with $d_V(x) < \eta/2$ there is a solution $\tilde{x} \in V$ such that $d_X(\tilde{x}, x) < \eta/2$. Moreover, for each $\tilde{x} \in V$ there is at most one $x \in V_J^{opt}$ such that $d_X(\tilde{x}, x) < \eta/2$. That follows from $d_X(x_1, x_2) \geq \eta$ for all distinct $x_1, x_2 \in V_J^{opt}$ and the triangle inequality of metric $d_X(\cdot,\cdot)$. In each iteration j of Step 2 holds $|V| < J$, therefore there exists a feasible solution $x \in V^*$ with $d_E(f(x)) \leq \delta^*$. Dual MDD optimization problem in Step 2 minimizes $d_E(f(x))$. Finally, in the last iteration of Step 3, $|V| = J$ and the proof follows. □

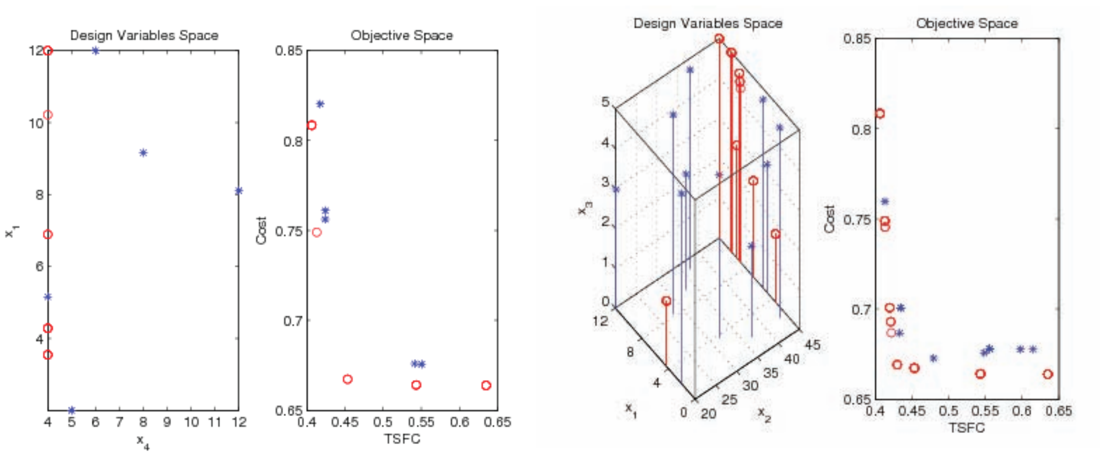
4. Computational Results

4.1 Model Description

To empirically assess the newly proposed algorithm, Algorithm 3.1 and DMA [3] were implemented using Matlab and AMPL with the COIN-OR Bonmin solver [1]. The use case of aircraft-engine design is formulated as a MINLP model, as provided by United Technologies Research Center (UTRC). This is a MINLP model with two objective functions: design cost (Cost) and fuel consumption (TSFC). There are 6 design variables, around 70 state variables and a few hundreds of constraints. The optimization problem is defined as follows: $minimize_{\{X\}} Cost\&TSFC$ subject to non-linear constraints and $x_i^{min} \leq x_i \leq x_i^{max}, i = 1 \dots 6, x_4$ is interger. Two experiments were conducted as described in the following sections.

4.2 Experiment 1

In the first experiment the performance of Algorithm 3.1 is compared to the performance of DMA. Since DMA was developed for an efficient-frontier exploration, the exploration of the design-variable space constitutes its byproduct. The goal is to find a set of the most diverse design-variable values. A weighted normalized Euclidean metric is defined for the x_1 and x_4 variables, with a greater weight for the integer variable. The results obtained by Algorithm 3.1 and DMA are depicted in Fig. 2(a) in blue stars and red circles, respectively. The left hand side (LHS) of the figure corresponds to the design-objective space and the right hand side (RHS) corresponds to the objective space. All the DMA solutions include $x_4 = 4$, whereas Algorithm 3.1 obtained five different samples for x_4. Also, it is evident that the projections of the latter onto the objective space are within 2% optimality violation from the efficient frontier. Overall, it is clear that Algorithm 3.1 obtained much higher diversity than DMA, as desired.



(a) (b)

Fig 2. (a) Experiment 1, (b) Experiment 2. LHS - design variables space, RHS - objective space. Red circles - DMA; Blue stars - Algorithm 3.1.

The straightforward extension of the aforementioned $2D$ case is the consideration of an additional design variable.

4.3 Experiment 2

A normalized Euclidean metric was defined for x_1, x_2 and x_3. The results obtained by Algorithm 3.1 and DMA, shown in Fig. 2(b), following the same tagging and partitioning as in Fig. 2(a). All but one DMA solutions are concentrated in one region, whereas the solutions attained by Algorithm 3.1 span the majority of the design-variable space. In addition, the projections of new solutions onto the objective space are within 5% optimality violation from the efficient frontier. Again, it is evident that Algorithm 3.1 obtained much higher diversity than DMA.

5. Discussion

After providing motivation for the problem of attaining maximal diversity within the design space for Multi-Objective optimization, Primal and Dual p-MDD problems were rigorously introduced and algorithms for solving them were presented. For the Primal p-MDD the proposed algorithm was proven to be a 2-approximation of the optimal algorithm and the upper bound of the optimality violation was computed with respect to the efficient frontier in the objective space. For the Dual p-MDD, the optimality violation of the proposed greedy algorithm was proven to be at least as good as that of the optimal algorithm when the lower bound on the distance between the solutions in the design-variable space is doubled. As an empirical demonstration of these algorithms, experiments on a real-world MINLP aircraft-engine design optimization problem were reported, in which a high diversity of solutions in the design-variable space was indeed accomplished, as desired. There are many interesting extensions of the MDD problem and potential algorithms. The authors intend to propose and analyze additional algorithms and different initial sets and distance functions in the journal-submission version of this paper.

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