A Note on Multiobjective Optimization and Complementarity Constraints^{*}

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Abstract

We propose a new approach to convex nonlinear multiobjective optimization that captures the geometry of the Pareto set by generating a discrete set of Pareto points optimally. We show that the problem of finding an optimal representation of the Pareto surface can be formulated as a mathematical program with complementarity constraints. The complementarity constraints arise from modeling the set of Pareto points, and the objective maximizes some quality measure of this discrete set. We present encouraging numerical experience on a range of test problem collected from the literature.

Keywords: Multiobjective optimization, nonlinear programming, complementarity constraints, mathematical program with complementarity constraints.

1 Introduction

We consider the solution of nonlinear multiobjective optimization problems (MOOPs). MOOPs arise in engineering and economic applications with multiple competing objectives. Applications include the construction of structures to minimize total mass and maximize stiffness, design problems with multiple loading cases, and airplane design to maximize fuel efficiency and minimize cabin noise; see the recent monographs [14, 22, 28, 31, 32].

The multiobjective optimization problem is formally defined as

$$(\text{MOOP}) \begin{cases} \min_{\substack{x \ge 0 \\ \text{subject to}}} & f(x) \\ \text{subject to} & c(x) \ge 0, \end{cases}$$

where $x \in \mathbb{R}^n$. We assume that the objective functions $f(x) = (f_1(x), \ldots, f_p(x)) : \mathbb{R}^n \to \mathbb{R}^p$ and that the constraints $c(x) = (c_1(x), \ldots, c_m(x)) : \mathbb{R}^n \to \mathbb{R}^m$ are twice continuously differentiable. We denote the feasible set by

$$\mathcal{F} := \{ x \ge 0 : c(x) \ge 0 \}$$

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and assume that it is nonempty.

We present a new approach to nonlinear multiobjective optimization that captures the geometry of the Pareto set by optimally generating a discrete set of Pareto points. We show that the problem of finding an optimal discrete representation of the Pareto set can be formulated as a bilevel optimization problem. If MOOP is convex, then we show how to solve the bilevel problem as a mathematical program with complementarity constraints (MPCC) by taking advantage of recent progress on the solution of MPCCs.

This paper is organized as follows: In the remainder of this section we review optimality conditions for MOOPs, discuss existing solution methods, and motivate our approach with a small example. The next section formally introduces our new approach and derives some theoretical properties of our formulation. Section 3 describes a random MOOP generator and a collection of test problems from the literature, and presents our numerical results.

1.1 Review of Multiobjective Optimization

We start by reviewing some basic concepts of MOOPs that will be used throughout the paper. Let x_k^* denote a solution to the single objective nonlinear program (NLP) given by

$$\begin{cases} \min_{\substack{x \ge 0 \\ \text{subject to} \\ c(x) \ge 0, \end{cases}} f_k(x) \tag{1.1}$$

and define the *payoff matrix* $Z \in \mathbb{R}^{p \times p}$ as $Z_{ij} := f_i(x_j^*)$, which provides useful information on the trade-offs between the multiple objectives. Note that the minima of each single objective NLP (1.1) are the diagonal of entries of Z and are also referred to as *ideal values*. The largest entry in each row is referred to as the *nadir values*. We define

$$\underline{z}^* := \left(f_1(x_1^*), \dots, f_p(x_p^*) \right) \text{ and } \overline{z}^* := \left(\max_{i \neq 1} f_1(x_i^*), \dots, \max_{i \neq p} f_p(x_i^*) \right)$$
(1.2)

and note that the ideal values \underline{z}^* and the nadir values \overline{z}^* give the range of the objective values.

Optimality conditions for MOOPs are given in [23], based on normal cones and Clarke's generalized gradients [4].

Definition 1.1 ([24]) Let $x^* \in \mathcal{F}$ be a feasible point with corresponding criterion vector $z^* = f(x^*)$.

- 1. (x^*, z^*) is globally Pareto optimal, if there exists no $x \in \mathcal{F}$, $x \neq x^*$ with $f_k(x) \leq f_k(x^*)$ for all $q = 1, \ldots, p$ and $f_r(x) < f_r(x^*)$ for at least one index $1 \leq r \leq p$.
- 2. (x^*, z^*) is locally Pareto optimal if there exists a $\delta > 0$ such that $x^* \in \mathcal{F}$ is globally Pareto optimal in $\mathcal{F} \cap B(x^*, \delta)$, where $B(x^*, \delta)$ is a ball of radius δ around x^* .
- 3. We designate the set of all Pareto points as $\mathcal{P} := \{z^* : (x^*, z^*) \text{ is a Pareto point}\}.$
- 4. MOOP is said to be convex if the functions f(x) and c(x) are convex.

The following result gives a necessary condition for local Pareto optimality.

Theorem 1.2 ([24]) Let $x^* \in \mathcal{F}$ be a feasible point at which Cottle's constraint qualification holds. A necessary condition for $z^* = f(x^*)$ to be locally Pareto optimal is that there exist multipliers $w \ge 0, w \ne 0$, and $y \ge 0$ such that

$$0 = \sum_{k=1}^{p} w_k \nabla f_k(x^*) - \sum_{j=1}^{m} y_j \nabla c_j(x^*)$$
(1.3)

and $y_j c_j(x^*) = 0$ for all j = 1, ..., m. If MOOP is convex, then this condition is also sufficient.

1.2 Solution Methods for MOOPs

Here, we briefly review two techniques for finding a single Pareto point. Both techniques form the basis of our approach to finding multiple Pareto points. The first technique forms a convex combination of the objective functions and solves the following NLP:

$$(\text{SUM}(w)) \begin{cases} \min_{x \ge 0} & \sum_{k=1}^{p} w_k f_k(x) \\ \text{subject to} & c(x) \ge 0, \end{cases}$$

where the weights $w_k \ge 0$, k = 1, ..., p with $\sum w_k = 1$. By choosing different weights we can identify different Pareto points.

The second technique is related to goal programming and classification techniques. It minimizes one objective subject to achieving a given goal on all other objectives. Without loss of generality, we let $f_1(x)$ be the objective that is minimized, and we denote the goals by $z \in \mathbb{R}^{p-1}$ and solve the following NLP:

$$(\text{GOAL}(z)) \begin{cases} \min_{\substack{x \ge 0 \\ \text{subject to} \\ c(x) \ge 0 \\ c(x) = 0$$

Clearly, the goals should be chosen to lie between the ideal and nadir vector, namely, $\underline{z}^* \leq (f_1(x), z) \leq \overline{z}^*$, though not all choices of z give rise to a feasible problem GOAL(z). We show in the next section that GOAL(z) gives rise to Pareto points.

1.3 Motivation of New Approach

One way in which we can obtain a discrete description of the Pareto set, \mathcal{P} , is to solve SUM(w) or GOAL(z) repeatedly for different weights or goals. However, choosing the weights and goals is not straightforward. For example, Das and Dennis have observed [6] that a uniform distribution of weights does not provide a uniform description of the Pareto set. Figure 1 shows two discrete descriptions of the Pareto set of three objective functions. The first description (green circles) was generated from a uniform distribution of the goals, while the second description (red boxes) was generated by maximizing the uniformity of the representation. Clearly, the optimized description provides a much better description of the Pareto set.

We close this section by summarizing our main assumptions.





Figure 1: Uniform Pareto set (green circles) and optimized Pareto set (red boxes)

Assumptions 1.3 Throughout we make the following assumptions:

- A1 The problem functions f(x) and c(x) are twice continuously differentiable.
- **A2** The feasible set $\mathcal{F} := \{x | x \ge 0 \text{ and } c(x) \ge 0\}$ is not empty and bounded.
- **A3** Any local solution to SUM(w) and GOAL(z) satisfies a linear independence constraint qualification and a second-order sufficient condition.
- A4 The functions f(x) and c(x) are convex.

Assumptions A1 to A3 are relatively weak, and simply ensure that any single objective NLP is tractable and can be solved by using standard NLP techniques. The most restrictive assumption is Assumption A4. The main reason for this assumption is that we replace the NLPs SUM(w) and GOAL(z) by their respective first-order conditions, which are necessary and sufficient, if the NLPs are convex.

2 Optimal Representation of the Pareto Surface

In this section we present a new approach to finding a discrete representation of the Pareto set, \mathcal{P} , that is optimal in a certain sense. We start by reviewing three quality measures of a discrete representations of the Pareto set proposed by Sayin [29] and show that they lead to a bilevel problem whose solution corresponds to an optimal representation of the Pareto set. We also derive a complementarity constraint formulation by replacing the lower level problems by their first-order conditions.

2.1 Bilevel Formulation of MOOPs

Sayin [29] introduces three quality measures of a discrete representations of the Pareto set: cardinality, coverage error, and uniformity of the representation. We assume here that the cardinality is user defined and is fixed. One can show that the coverage error requires explicit knowledge of the complete Pareto set and is therefore not a practical measure of quality. Thus, the only practical way of measuring the quality of a representation of the Pareto set is the uniformity of the representation, which is defined as the largest η such that

$$\eta \le \min_{u,v \in \mathcal{D}, \ u \ne v} \|u - v\|,\tag{2.4}$$

where $\mathcal{D} \subset \mathcal{P}$ is a discrete representation of the Pareto set \mathcal{P} .

Next, we show that the problem of finding a maximal uniform representation of the Pareto set \mathcal{P} can be formulated as a bilevel programming problem. The key idea is to take *any* single solution approaches SUM(w) or GOAL(z) and to let the weights or goals be variables to be determined within a bilevel optimization problem. The upper level aims to maximize the quality of the representation of the Pareto set, while the lower level corresponds to (a finite number of) single solution NLPs.

Figure 2 provides a graphical illustration of our approach. There are two objective functions, and the solid line shows the Pareto set. We are seeking a given number of discrete points such that the pairwise distances between the Pareto points is maximized, illustrated by the circles around each Pareto point. Here, we maximize η subject to the constraints $\eta \leq \eta_{lk}$, where $\eta_{lk} = ||f(x_l) - f(x_k)||$, and x_l are Pareto points characterized by solving SUM(w) or GOAL(z).



Figure 2: Maximizing distances between Pareto points

Formally, we consider the problem of finding a given number q of Pareto points that maximize the uniformity of the discrete representation of the Pareto set. We start by deriving a problem to find an optimal representation of the Pareto set based on the convex combination problem SUM(w). Let $w := (w_1, \ldots, w_q)^T$ denote the weights to be determined, and let $x := (x_1, \ldots, x_q)^T$ denote the corresponding Pareto points (one copy for each Pareto point). The problem of maximizing the uniformity of the discrete representation of the Pareto set can then be formulated as the following bilevel optimization problem:

$$\begin{cases} \underset{x,w,\eta}{\text{maximize}} & \eta\\ \text{subject to} & \eta \leq \|f(x_l) - f(x_k)\|_2^2 & \forall \ 1 \leq k, l \leq q, \ k \neq l\\ & w_k \geq 0, \text{ and } e^T w_k = 1, \ \forall \ k = 1, \dots, q\\ & x_k \text{ solves SUM}(w_k). \end{cases}$$
(2.5)

The aim (2.5) is to find $q \ge 2$ Pareto points such that the smallest distance between any two function values f_k is pushed as far apart as possible while remaining within the Pareto set. As is customary in bilevel optimization, we refer to w and η as the control, or upper-level, variables and to x as the state, or lower-level, variables. We note that even though MOOP is convex, the bilevel problem is in general nonconvex, and the task of finding a global solution is daunting. However, we will show in Section 3 that even local solutions of (2.5) provide improved representations of the Pareto set.

One disadvantage of (2.5) is the lack of general-purpose solvers for bilevel optimization problems. To develop a practical technique for solving (2.5), we therefore replace the constraint " x_k solves $SUM(w_k)$ " by its first-order conditions, and exploit recent advances in the development of robust solvers for mathematical programs with complementarity constraints.

Under Assumptions A1–A4, it follows that the first-order conditions for $SUM(w_k)$ are necessary and sufficient, and we can therefore equivalently replace (2.5) by the following mathematical program with complementarity constraints (MPCC):

$$\begin{cases} \underset{x,y,w \ge 0,\eta}{\text{subject to}} & \eta \\ \text{subject to} & \eta \le \|f(x_k) - f(x_l)\|_2^2 & \forall \ 0 \le k, l \le q \ , \ k \ne l \\ e^T w_l = 1 & \forall \ l = 1, \dots, q \\ 0 \le x_l \perp \nabla \left(w_l^T f(x_l)\right) - \nabla c(x_l) y_l \ge 0 & \forall \ l = 1, \dots, q \\ 0 \le y_l \perp c(x_l) \ge 0 & \forall \ l = 1, \dots, q, \end{cases}$$
(2.6)

where \perp is the usual MPCC complementarity condition and means that $y_l^T c(x_l) \leq 0$. We note that the dimension of (2.6) is roughly q times the dimension of SUM (w_l) , as every Pareto point requires a new copy of the primal and dual variables x and y. We can remove one component of each w_l and the constraints $e^T w_l = 1$ if we replace the first-order condition by

$$0 \le x_l \perp \nabla \left((1, \hat{w}_l)^T f(x_l) \right) - \nabla c(x_l) y_l \ge 0 \ \forall l = 1, \dots, q,$$

$$(2.7)$$

where $\hat{w}_l \in \mathbb{R}^{p-1}$ are the weights on the remaining objectives. This formulation has the advantage that it removes one bilinearity from the first-order condition.

An alternative MPCC is obtained by using the first-order conditions of GOAL(z). In this case, we are looking for goals $z = (z_1, \ldots, z_q)$ and corresponding multipliers u =

 (u_1,\ldots,u_q) that solve

$$\begin{cases} \underset{x,y,z,u,\eta}{\text{maximize}} & \eta \\ \text{subject to} & \eta \leq \|f(x_k) - f(x_l)\|_2^2 & \forall 0 \leq k, l \leq q, \ k \neq l \\ & 0 \leq x_l \perp \nabla \left((1, u_l)^T f(x_l)\right) - \nabla c(x_l) y_l \geq 0 & \forall l = 1, \dots, q \\ & 0 \leq y_l \perp c(x_l) \geq 0 & \forall l = 1, \dots, q \\ & 0 \leq u_l \perp \hat{f}(x_l) \leq z_l, \end{cases}$$

$$(2.8)$$

where $\hat{f}(x_l) = (f_2(x_l), \ldots, f_p(x_l))$. We note that even if the MOOP is linear, the MPCCs (2.6) and (2.8) are nonconvex optimization problems, because of the presence of the complementarity constraints and the upper bound on $\eta \leq ||f(x_k) - f(x_l)||_2^2$. Thus, in practice we can at best hope to find a local solution.

Numerical experience has shown that it can be advantageous to work with a componentwise definition of η . Thus, the goal programming version becomes

$$\begin{cases} \underset{x,y,z,u,\eta}{\operatorname{maximize}} & \sum_{i=1}^{p} \eta_{i} \\ \text{subject to} & \eta_{i} \leq |f_{i}(x_{k}) - f_{i}(x_{l})|^{2} & \forall 0 \leq k, l \leq q, \ k \neq l \\ & \text{and} \ \forall i = 1, \dots, p \\ 0 \leq x_{l} \perp \nabla \left((1, u_{l})^{T} f(x_{l}) \right) - \nabla c(x_{l}) y_{l} \geq 0 \quad \forall l = 1, \dots, q \\ 0 \leq y_{l} \perp c(x_{l}) \geq 0 & \forall l = 1, \dots, q \\ 0 \leq u_{l} \perp \widehat{f}(x_{l}) \leq z_{l}. \end{cases}$$

$$(2.9)$$

Similarly we can define componentwise versions with the first-order conditions of $SUM(w_k)$. This new MPCC approach can be generalized easily by using other single objective characterizations of Pareto points. Many algorithmic choices and variants are possible and can be used to tackle multiobjective optimization problems within the framework of equilibrium constraints.

2.2 Theoretical Foundation of New Approach

We start by recalling that under Assumptions A1–A4, the first-order conditions of SUM(w) and GOAL(z) characterize a Pareto point. This result is a direct corollary of Theorem 1.2.

Corollary 2.1 Let Assumption A1–A4 hold. Then it follows that (x^*, y^*) is a Pareto point if

- 1. (x^*, y^*) solve the first-order conditions of SUM(w) for some weights $w \ge 0$ with $e^T w = 1$, or if
- 2. (x^*, y^*, u^*) solve the first-order conditions of GOAL(z) for some goals z.

Next, we show that the solution of the bilevel program (2.5) gives rise to a set of Pareto points.

Proposition 2.2 Let the Assumption A1–A4 hold. Then it follows that

1. if $(x_k^*, y_k^*, w_k^*, \eta^*)$ solves problem (2.6), then (x_k^*, f_k^*) are Pareto points of MOOP;

2. if $(x_k^*, y_k^*, u_k^*, z_k^*, \eta^*)$ solves problem (2.8), then (x_k^*, f_k^*) are Pareto points of MOOP. Moreover, in each case, if η^* is the global maximizer, then η^* maximizes the uniformity of the discrete representation of the Pareto set.

What makes this new approach practical is the fact that the MPCCs can be solved reliably and efficiently as nonlinear programs (NLPs) [1, 11]. For example, a suitable NLP formulation of the MPCC (2.6) is given by

where we have introduced slacks to obtain a numerically favorable formulation. It is well known that (2.10) violates the Mangasarian-Fromowitz constraint qualification at any feasible point [3] because of the presence of the bilinear terms $x_l^T s_l \leq 0$ and $y_l^T t_l \leq 0$. Recently, however, it has been shown [11] that any stationary point of the NLP (2.10) is a strongly stationary point [30] of the MPCC (2.6) and vice versa. This fact has been used to show that standard NLP solvers can tackle MPCCs reliably and efficiently [1, 2, 11, 10, 18, 19, 21, 27]. We note that similar results hold for other nonlinear formulations of the complementarity conditions [17].

One limitation of our approach is the fact that even linear MOOPs such as

$$\begin{cases} \begin{array}{ll} \underset{x}{\text{maximize}} & C^T x\\ \text{subject to} & A^T x \ge b\\ & x > 0 \end{array} \end{cases}$$

lead to nonconvex NLP formulations. The reason for the nonconvexity of (2.6) is the presence of the constraints $\eta \leq ||C^T x_k - C^T x_l||_2^2$ and the presence of the complementarity constraints. Thus, in general we cannot expect to find the global minimum of (2.6). However, numerical experience presented in the next section shows that our approach is promising.

Another limitation of our approach is the requirement that the MOOP must be convex (Assumption A4). Consider the following MOOP:

minimize
$$[(x^2 - 1)^2, (x^2 - 4)^2].$$
 (2.11)

It follows that $f_1(x)$ has two minimizers at $x = \pm 1$ and a maximum at x = 0. Likewise, $f_2(x)$ has two minimizers at $x = \pm 2$ and a maximum at x = 0. However, the MPCC (2.6) cannot distinguish between minima and maxima. Thus, one solution is $x_1 = 1$ and $x_2 = 0$ at which $\eta = 81$ is maximized. Clearly, x = 0 is not a Pareto point, but the objective in MPCC (2.6) is maximized if one of the two "Pareto points" found by (2.6) is a maximizer and the other is a minimizer. Note that we could still use the bilevel formulation (2.5), but that would rule out the use of standard NLP solvers.

3 Numerical Experience

This section presents our numerical results. To test our approach, we have collected test problems from the literature and generated random quadratic MOOPs. All test problems and the random generator are available at www.mcs.anl.gov/~leyffer/MOOP/.

3.1 Obtaining Good Starting Points

Early numerical experience showed that the NLP solvers may fail to find a feasible point to the MPCC formulations (2.6) or (2.8). Hence we have adopted the following strategy for finding initial feasible points. We first fix the weights, or goals and solve the resulting NCP using PATH. This is a standard strategy for solving complex MPCCs and is readily implemented in AMPL by ng the named model facility.

Another difficulty that arose for some problems is that different weights can give rise to the same Pareto point. Unfortunately, this corresponds to a stationary point of the MPCC (2.6) and (2.8) with $\eta^* = 0$. Thus we ran the NCP solver for different choices of weights until we found a set of Pareto points with $\eta \neq 0$. This initial NCP solution also provides an initial guess at the maximum uniformity.

3.2 Description of Test Problems and Solvers

Table 1 shows the name of the test problem, the number of variables, n, the number of constraints m, the number of objectives p, and the source and describes the nonlinearity of the problem. We note that our collection also contains nonconvex problems, namely, ABC-comp, ex002, and ex004.

Name	n	m	p	Source	Problem Type
ABC-comp	2	3	2	[16]	quadratic objective & bilinear constraints
ex001	5	3	2	[5]	quadratic objective & constraints
ex002	5	2	2	[34]	quadratic objective & nonlinear constraints
ex003	2	2	2	[33]	quadratic objective & nonlinear constraints
ex004	2	3	2	[26]	nonlinear objective & linear constraints
ex005	2	0	2	[16]	nonlinear objective & bounds
hs05x	5	3	3	[15] [own]	quadratic objective & linear constraints
liswetm	7	5	2	[20] [own]	quadratic objective & linear constraints
MOLPg-1	8	8	3	[32]	linear objective and constraints
MOLPg-2	12	16	3	[32]	linear objective and constraints
MOLPg-3	10	14	3	[32]	linear objective and constraints
MOQP[01-03]	20	10	3	[own]	quadratic objective & linear constraints

Table 1: Multiobjective Optimization Problem Characteristics

Problems hs05x and liswetm are constructed from several academic NLP test problems that have the same constraints and different objective functions. We have also written a random MOOP generator that generates multiobjective quadratic programs with linear constraints. The generator is written in matlab and can generate large sparse problems.

The Hessian matrix is forced to be positive definite by adding a suitably large multiple of the identity to the diagonal. This ensures that the resulting MOOPs are convex.

Table 2 shows the size of the NCP and the various MPCC formulations for q = 10 Pareto points. Here, n, m, and r refer to the number of variables, the number of constraints, and the number of complementarity conditions, respectively. As expected, the growth in terms of the number of variables compared to the NCP formulation is modest, while the increase in the number of constraints corresponds to the addition of the constraints $\eta \leq \ldots$, which is of order q^2 . We also note that formulation (2.8) gives rise to the largest MPCCs because we have added multipliers of the goal constraints.

		NCP			(2.6)			(2.7)			(2.8)	
name	$\mid n \mid$	m	r	$\mid n$	m	r	$\mid n$	m	r	n	m	r
ABC-comp	51	51	50	71	105	50	61	95	50	71	150	60
ex001	80	80	10	101	135	10	91	125	10	101	180	20
ex002	70	70	50	91	134	50	81	115	50	91	170	60
ex003	40	40	40	61	104	40	51	94	40	61	140	50
ex004	40	40	40	61	104	40	51	94	40	51	130	40
ex005	20	20	20	41	84	20	31	74	20	41	120	30
hs05x	80	80	50	111	135	50	101	170	50	121	190	70
liswetm	121	121	50	141	184	50	131	174	50	141	220	60
MOLPg-1	160	160	160	191	260	160	181	250	160	201	290	160
MOLPg-2	291	291	280	321	390	280	311	380	280	331	420	280
MOLPg-3	261	261	240	291	360	240	281	350	240	301	390	240
MOQP[01-03]	311	311	300	341	410	300	331	400	300	351	420	320

Table 2: Characteristics of NCP, and MPCC Formulations

The problems are formulated in AMPL [13], and the initial NCPs are solved by using PATH [7, 8]. PATH implements a generalized Newton method that solves a linear complementarity problem to compute the search direction. The MPCCs are solved by using filterSQP [9, 10] which automatically reformulates the complementarity constraints as nonlinear equations. This solver implements a sequential quadratic programming algorithm with a filter to promote global convergence [12].

3.3 Detailed Numerical Results

Table 3 summarizes our numerical experience. The table shows the number of major (Newton) iterations and the final value of η , which can be taken as an indication of the quality of the computed representation of the Pareto set. We provide results only for the NCP version of SUM(w); results for the other formulations are similar, and we merely mention the NCP run to illustrate the start-up cost and the improvement in uniformity that can be achieved. The iteration limit for all solvers is 1,000 major iterations.

Failures of the solvers are indicated by the following code: [S] indicates termination with segmentation fault; [I] means that the solver failed to find a feasible point. Unfortunately, this latter outcome is difficult to avoid because the MPCC are nonconvex. In our

	NCP			(2.6)		(2.7)	(2.8)			
name	iter	η^*	iter	η^*	iter	η^*	iter	η^*		
ABC-comp	5	1.154	44	28.43	11	28.43	36	[I]		
ex001	4	1.210E-2	28	1.648	14	1.648	4	1.648		
ex002	22	4.723E-7	21	3.245E-6	78	$2.107 \; [L]$	45	$3.206 \ [L]$		
ex003	23	1.944E-6	22	2.912E-4	11	4.478E-1	1	8.449 E-2		
ex004	6	3.577E-2	14	6.441E-1	49	6.441E-1	13	8.150E-1 [L]		
ex005	2	8.702E-5	405	1.656E-2	1000	1.540E-2	9	1.496E-1		
hs05x	1	1.615E-1	237	323.2	374	323.3	193	316.5		
listwetm	0	1.847E-2	48	2.830E-1	217	2.830E-1	62	2.210E-4		
MOLPg-1	7	0	1	0	1	0	10	52.11		
MOLPg-2	5	0	4	0	6	0	18	3.623		
MOLPg-3	7	0	5	0	7	0	24	15.74		
MOQP-01	6	243.3	296	5466	897	5622	452	3117		
MOQP-02	[S]		262	4046	1000	[I]	707	5235		
MOQP-03	9	69.66	1000	[I]	1000	[I]	488	1160		

Table 3: Numerical Results for NCP and MPCC Formulations

experience, warm-starting the MPCCs from a solution of the initial NCP greatly improves the likelihood of finding a feasible MPCC solution. Runs for which the solver failed to converge within the limit of 1,000 iterations are identified by 1,000 in the iter column. We note that for only two problems does the solver fail in this way, namely, ex005 and MOQP-3.

The results for the nonconvex MOOPs are interesting. As indicated earlier (see (2.11)), nonconvex MOOPs can have the undesirable effect of increasing η by placing points x_k at local maxima. This failure, indicated by [L], occurs on the two nonconvex examples (ex002 and ex004). Figure 3 shows the computed Pareto set for ex004. Despite the fact that we identify some spurious Pareto points, the figure still provides useful information on the Pareto set. Moreover, for the nonconvex example ABC-comp, we are able to find valid approximations of the Pareto set.

The results in Table 3 show that the MPCC formulation based on goal programming, (2.8), is clearly superior to the other two formulations: the formulation based on goal programming is the only formulation that achieves positive separation between all Pareto points for the MOLPg problems. In addition, it is up to an order of magnitude faster than the formulations based on the convex sum. We believe that in general, goal programming is a better way to generate a uniform set of Pareto points because the control on the objective is more direct through the goal constraints.

4 Conclusions and Outlook

We have presented a new approach to solving multiobjective optimization problems that finds a maximally uniform representation of the Pareto set. We show how this problem can be formulated as a mathematical program with complementarity constraints, and we



Figure 3: Pareto set with spurious points for ex004

present three different formulations based on convex sum and goal-programming single objective formulations of MOOP. Preliminary numerical results are encouraging, especially for the approach based on goal programming.

Our new MPCC approach can be generalized easily by using other single objective characterizations of Pareto points. Many algorithmic choices and variants are possible and can be used to tackle multiobjective optimization problems within the framework of equilibrium constraints. More numerical experience is needed to decide which of these schemes works best under which circumstances.

Important open questions do remain, however. For example, the reformulation requires the user to form the first-order conditions of a single-objective formulation of MOOP, a process that (from our experience) is prone to error. In addition, the first-order conditions are necessary and sufficient only if the MOOP is convex. We have observed examples where a lack of convexity results in spurious Pareto points being found by our approach.

Some of these limitations can be overcome by better MPCC solvers that preserve local minima. However, such an approach would make it harder to exploit the available NLP solver technology. The requirement that the user form first-order conditions can be overcome by developing extensions to AMPL that allow bilevel optimization models. However, this is a nontrivial task because AMPL would then have to provide derivatives up to third order for the Hessian matrices used in the NLP solvers.

Ultimately, we believe that our technique can be incorporated into interactive MOOP solution approaches such as www-nimbus [25]. The advantage of our approach is that it provides a broader picture of the Pareto set. By allowing the user to interact with this representation, we believe that our approach can be made more robust and less susceptible to problems caused by nonconvexities.

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References

- M. Anitescu. Global convergence of an elastic mode approach for a class of mathematical programs with complementarity constraints. SIAM J. Optimization, 16(1):120– 145, 2005.
- [2] H. Benson, D. F. Shanno, and R. V. D. Vanderbei. Interior-point methods for nonconvex nonlinear programming: Complementarity constraints. Technical Report ORFE 02-02, Princeton University, Operations Research and Financial Engineering, 2002.
- [3] Y. Chen and M. Florian. The nonlinear bilevel programming problem: Formulations, regularity and optimality conditions. *Optimization*, 32:193–209, 1995.
- [4] F.H. Clarke. Optimization and Nonsmooth Analysis. Wiley, New York, 1983 (reprinted by SIAM, 1990).
- [5] I. Das and J. E. Dennis. A closer look at drawbacks of minimizing weighted sums of objectives for pareto set generation in multicriteria optimization problems. Dept. of CAAM Tech. Report TR-96-36, Rice University, Houston, TX, December 1996.
- [6] I. Das and J. E. Dennis. Normal-boundary intersection: A new method for generating the Pareto surface in nonlinear multicriteria optimization problems. SIAM Journal on Optimization, 8(3):631–657, August 1998.
- [7] S. P. Dirkse and M. C. Ferris. The path solver: A non-monotone stabilization scheme for mixed complementarity problems. *Optimization Methods and Software*, 5:123–156, 1995.
- [8] M. C. Ferris and T. S. Munson. Complementarity problems in GAMS and the PATH solver. Journal of Economic Dynamics and Control, 24(2):165–188, 2000.
- [9] R. Fletcher and S. Leyffer. Nonlinear programming without a penalty function. Mathematical Programming, 91:239–270, 2002.
- [10] R. Fletcher and S. Leyffer. Solving mathematical program with complementarity constraints as nonlinear programs. *Optimization Methods and Software*, 19(1):15–40, 2004.
- [11] R. Fletcher, S. Leyffer, D. Ralph, and S. Scholtes. Local convergence of SQP methods for mathematical programs with equilibrium constraints. Numerical Analysis Report NA/209, Department of Mathematics, University of Dundee, Dundee, UK, May 2002.
- [12] R. Fletcher, S. Leyffer, and Ph. L. Toint. On the global convergence of a filter-SQP algorithm. SIAM J. Optimization, 13(1):44–59, 2002.
- [13] R. Fourer, D. M. Gay, and B. W. Kernighan. AMPL: A Modelling Language for Mathematical Programming. Books/Cole—Thomson Learning, 2nd edition, 2003.
- [14] C. Hillermeier. Nonlinear Multiobjective Optimization. Birkhäuser Verlag, Berlin, 2001.

- [15] W. Hock and K. Schittkowski. Test Examples for Nonlinear Programming Codes. Springer-Verlag, Berlin, 1981.
- [16] C.-L. Hwang and A.S.M. Masud. Multiple Objective Decision Making Methods and Applications, volume 164 of Lecture Notes in Economics and Mathematical Systems. Springer-Verlag, Berlin, 1979.
- [17] S. Leyffer. Complementarity constraints as nonlinear equations: Theory and numerical experience. Preprint ANL/MCS-P1054-0603, Argonne National Laboratory, Argonne, IL, September 2003.
- [18] S. Leyffer. Mathematical programs with complementarity constraints. SIAG/OPT Views-and-News, 14(1):15–18, 2003.
- [19] S. Leyffer, G. Lopez-Calva, and J. Nocedal. Interior methods for mathematical programs with complementarity constraints. Preprint ANL/MCS-P1211-1204, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, 2004.
- [20] W. Li and J. Swetits. A Newton method for convex regression, data smoothing and quadratic programming with bound constraints. SIAM J. Optimization, 3(3):466– 488, 1993.
- [21] X. Liu, G. Perakis, and J. Sun. A robust SQP method for mathematical programs with linear complementarity constraints. Technical report, Department of Decision Sciences, National University of Singapore, 2003.
- [22] K. Miettinen. Nonlinear Multiobjective Optimization. Kluwer Academic Publishers, Boston, 1999.
- [23] K. Miettinen and M. M. Mäkelä. Proper Pareto optimality in nonconvex problems – characterization with tangent and normal cones. Report 11/1998, University of Jyväskylä, Dept. of Mathematics, P.O. Box 35, FIN-40351, Finland, 1998.
- [24] K. Miettinen and M. M. Mäkelä. Theoretical and computational comparison of multiobjective optimization methods NIMBUS and RD. Report 5/1998, University of Jyväskylä, Dept. of Mathematics, P.O. Box 35, FIN-40351, Finland, 1998.
- [25] K. Miettinen and M. M. Mäkelä. Interactive multiobjective optimization system WWW-NIMBUS on the internet. Computers & Operations Research, 27:709–723, 2000.
- [26] S. L. C. Oliveira and P. A. V. Ferreira. Bi-objective optimization with multiple decision-makers: a convex approach to attain majority solutions. *JORS*, 51:333–340, 2000.
- [27] A. Raghunathan and L. T. Biegler. Barrier methods for mathematical programs with complementarity constraints (MPCCs). Technical report, Carnegie Mellon University, Department of Chemical Engineering, Pittsburgh, PA, December 2002.

- [28] B. Rustem. Algorithms for Nonlinear Programming and Multiple Objective Decision. Wiley, Chichester, 1998.
- [29] S. Sayin. Measuring the quality of discrete representations of efficient sets in multiple objective mathematical programming. *Mathematical Programming*, 87(3):543–560, May 2000.
- [30] H. Scheel and S. Scholtes. Mathematical program with complementarity constraints: Stationarity, optimality and sensitivity. *Mathematics of Operations Research*, 25:1– 22, 2000.
- [31] W. Stadler, editor. *Multicriteria Optimization in Engineering and in the Sciences*. Plenum Press, New York, 1988.
- [32] R. E. Steuer. Multiple Criteria Optimization: Theory, Computation and Applications. John Wiley & Sons, New York, 1986.
- [33] R. V. Tappeta and J. E. Renaud. Interactive multiobjective optimization procedure with local preferences. In *Proceedings of the 3rd WCSMO*, Buffalo, New York, May 1999. http://www.eng.buffalo.edu/Research/MODEL/wcsmo3/proceedings/.
- [34] J.-F. Wang and J. E. Renaud. Automatic differentiation in multi-objective collaborative optimization. In *Proceedings of the 3rd WCSMO*, Buffalo, New York, May 1999. http://www.eng.buffalo.edu/Research/MODEL/wcsmo3/proceedings/.

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