A Complementarity Constraint Formulation of Convex Multiobjective Optimization Problems

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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 a maximally uniform 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 problems collected from the literature.

Key words: multiobjective optimization; nonlinear programming; complementarity constraints; mathematical program with complementarity constraints

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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 (Ehrgott 2005, Hillermeier 2001, Miettinen 1999, Rustem 1998, Stadler 1988, Steuer 1986).

The multiobjective optimization problem is formally defined as

\[
\text{(MOOP)} \quad \begin{cases} 
\text{minimize} & f(x) \\
\text{subject to} & c(x) \geq 0,
\end{cases}
\]

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

\[
\mathcal{F} := \{ x \geq 0 : c(x) \geq 0 \}
\]

and assume that it is nonempty.

We present a new approach to nonlinear multiobjective optimization that captures the geometry of the Pareto set by generating a discrete set of Pareto points that maximizes the uniformity of the representation of the Pareto set. 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 (MPCCs) by taking advantage of recent progress on the solution of MPCCs.

This paper is organized as follows. In the remainder of this section we briefly review optimality conditions for MOOPs, discuss existing solution methods, and motivate our approach with a small example. In §2 we formally introduce our new approach and derive some theoretical properties of our formulation. In §3 we describe a random MOOP generator and a collection of test problems from the literature, and we present our numerical results. In §4 we briefly examine open questions and suggest some future lines of research.

1.1. Introduction to 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

\[
\begin{align*}
\text{minimize} & \quad f_k(x) \\
\text{subject to} & \quad c(x) \geq 0,
\end{align*}
\]

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) are the diagonal of entries of \( Z \), also referred to as ideal values. We define

\[
\begin{align*}
    z^* := (f_1(x_1^*), \ldots, f_p(x_p^*)) \quad \text{and} \\
    \bar{z}^* := \left( \max_{i \neq p} f_i(x_i^*), \ldots, \max_{i \neq p} f_p(x_p^*) \right),
\end{align*}
\]

and note that the ideal values \( z^* \) and the maximum values \( \bar{z}^* \) approximate the range of the objective values.

Optimality conditions for MOOPs are given by Miettinen and Mäkelä (1998a), based on normal cones and Clarke’s generalized gradients (Clarke 1983).

**Definition 1.1** (Miettinen and Mäkelä 1998b). Let \( x^* \in \mathcal{F} \) be a feasible point with the 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 \( k = 1, \ldots, p \), 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 \( \delta \) 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 \( f(x) \) are convex and the constraint functions \( c(x) \) are concave (i.e., the feasible set is convex).

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

**Theorem 1.2** (Miettinen and Mäkelä 1998b). 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 \( w \geq 0, w \neq 0, \) and \( y \geq 0 \) such that

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

and \( y_j c(x^*) = 0 \) for all \( j = 1, \ldots, m \). 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. Other techniques can be found in recent monographs by Ehrigott (2005) and Miettinen (1999). 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:

\[
\begin{align*}
    \text{(SUM}(w) \text{)} \quad \text{minimize} & \quad \sum_{k=1}^p w_k f_k(x) \\
    \quad \text{subject to} & \quad c(x) \geq 0,
\end{align*}
\]

where the weights \( w_k \geq 0, k = 1, \ldots, p \), with \( \sum w_k = 1 \). By varying the weights we can identify different Pareto points. We are grateful to an anonymous referee for pointing out that \( \text{SUM}(w) \) may generate weakly dominated solutions. Only if the MOOP is convex can \( \text{SUM}(w) \) generate all Pareto points by varying \( w \).

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:

\[
\begin{align*}
    \text{(GOAL}(z) \text{)} \quad \text{minimize} & \quad f_1(x) \\
    \quad \text{subject to} & \quad f_k(x) \leq z_k, k = 2, \ldots, p, \\
    & \quad c(x) \geq 0.
\end{align*}
\]

Clearly, the goals should be chosen to lie between \( z^* \) and \( \bar{z}^* \), although not all choices of \( z \) give rise to a feasible problem \( \text{GOAL}(z) \). We show in the next section that \( \text{GOAL}(z) \) gives rise to Pareto points. In contrast to \( \text{SUM}(w) \), however, all feasible choices of target \( z \) generate a Pareto point, and all Pareto points can be found by varying \( z \).

**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 \( \text{SUM}(w) \) or \( \text{GOAL}(z) \) repeatedly for different weights or goals. However, choosing the weights and goals is not straightforward. For example, Das and Dennis (1998) have observed 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 (circles) was generated from a uniform distribution of the goals, while the second description (boxes) was generated by maximizing the uniformity of the representation. The figure shows two viewpoints of the same three-dimensional (3-D) Pareto set and shows that the optimized description provides a better description of the Pareto set.

We close this section by summarizing our main assumptions.

**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 \( \mathcal{F} := \{ x \mid x \geq 0 \text{ and } c(x) \geq 0 \} \) is not empty and bounded.

A3. Any local solution to \( \text{SUM}(w) \) and \( \text{GOAL}(z) \) satisfies the Mangasarian-Fromowitz 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. We could replace the boundedness assumption A2 by an assumption on the boundedness of level sets of an exact penalty function. The most restrictive assumption is Assumption A4. The main reason for this assumption is that we replace the NLPs SUM and GOAL by their respective first-order conditions, which are necessary and sufficient, if the NLPs are convex. We note that convexity does not imply the second-order sufficient condition.

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 representation of the Pareto set proposed by Sayin (2000) 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 (2000) introduces three quality measures of a discrete representation of the Pareto set: cardinality, coverage error, and uniformity of the representation. We assume here that the cardinality is user defined and is fixed. The coverage error for a discrete representation \( \mathcal{D} \subset \mathcal{P} \) of the Pareto set, \( \mathcal{P} \), is defined as

\[
\epsilon = \max_{v \in \mathcal{P}} \min_{u \in \mathcal{D}} \| u - v \|,
\]

where \( \| \cdot \| \) is any norm in \( \mathbb{R}^p \). Unfortunately, to compute this measure, we require explicit knowledge of the Pareto set, \( \mathcal{P} \). We therefore believe that coverage error is not a practical measure of quality. However, the final quality measure introduced by Sayin (2000) — namely, the uniformity of the representation — can be used to derive optimally uniform approximations of the Pareto set. Uniformity of representation is defined as the largest \( \eta \) such that

\[
\eta \leq \min_{u, v \in \mathcal{P}, u \neq v} \| u - v \|.
\]

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. We consider any single-objective approach such as SUM \( w \) or GOAL \( z \) and consider the parameters \( w \) or \( z \) as variables that are optimally determined within a bilevel optimization problem. The key idea is to simultaneously determine \( q \geq 2 \) Pareto points \( x_i \) for \( l = 1, \ldots, q \), and their corresponding parameters \( w_l \) (or \( z_l \)) such that the Pareto points maximize the uniformity of the presentation of the Pareto set. The upper level controls the parameters \( w_l \) (or \( z_l \)), while the lower level corresponds to \( q \) single-objective NLPs given by \( \text{SUM}(w_l) \) or \( \text{GOAL}(z_l) \).

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 \( \eta \) subject to the constraints \( \eta \leq \eta_{kl} \), where \( \eta_{kl} = \| f(x_{kl}) - f(x_l) \| \) and \( x_l \) are Pareto points characterized by solving \( \text{SUM}(w_l) \) or \( \text{GOAL}(z_l) \).

Formally, we consider the problem of finding a given number \( q \geq 2 \) 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 \( \text{SUM}(w) \). 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 (in the remainder we choose the $\ell_2$ norm for simplicity):

$$\begin{align*}
\text{maximize} & \quad \eta \\
\text{subject to} & \quad \eta \leq \|f(x_i) - f(x_k)\|_2^2 \\
& \quad \forall 1 \leq k, l \leq q, k \neq l, \\
& \quad w_k \geq 0, \text{ and } e^T w_k = 1, \quad \forall k = 1, \ldots, q, \\
& \quad x_k \text{ solves } \text{SUM}(w_k).
\end{align*}$$

The aim in (5) is to find $q \geq 2$ 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 $\eta$ 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 present numerical evidence in §3 that even local solutions of (5) provide improved representations of the Pareto set.

One disadvantage of (5) is the lack of general-purpose solvers for bilevel optimization problems. To develop a practical technique for solving (5), we therefore replace the constraint “$x_k$ solves $\text{SUM}(w_k)$” 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 $\text{SUM}(w_k)$ are necessary and sufficient. We can therefore equivalently replace (5) by the following mathematical program with complementarity constraints (MPCC):

$$\begin{align*}
\text{maximize} & \quad \eta \\
\text{subject to} & \quad \eta \leq \|f(x_i) - f(x_k)\|_2^2 \\
& \quad \forall 0 \leq k, l \leq q, k \neq l, \\
& \quad e^T w_l = 1 \quad \forall l = 1, \ldots, q, \\
& \quad 0 \leq x_l \perp \nabla(w_l^T f(x_l)) - \nabla(c(x_l)) y_l \geq 0 \\
& \quad \forall l = 1, \ldots, q, \\
& \quad 0 \leq y_l \perp c(x_l) \geq 0 \quad \forall l = 1, \ldots, q,
\end{align*}$$

where the last two sets of constraints are complementarity constraints. The notation $0 \leq u \perp v \geq 0$ means that the two vectors $u, v \geq 0$ and that, in addition, $u^T v \leq 0$; that is, a component $i$ of $u_i = 0$ or the corresponding component of $v_i = 0$. We note that the dimension of (6) is roughly $q$ times the dimension of $\text{SUM}(w_l)$ (plus $q \times p$ weights), 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

$$0 \leq x_l \perp \nabla((1, \hat{w}_l)^T f(x_l)) - \nabla(c(x_l)) y_l \geq 0$$

$$\forall l = 1, \ldots, q,$$

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. We note, however, that (6) and (7) are not equivalent, because the latter overemphasizes the first objective.

An alternative MPCC is obtained by using the first-order conditions of $\text{GOAL}(z)$. 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

$$\begin{align*}
\text{maximize} & \quad \eta \\
\text{subject to} & \quad \eta \leq \|f(x_i) - f(x_k)\|_2^2 \\
& \quad \forall 0 \leq k, l \leq q, k \neq l, \\
& \quad 0 \leq x_l \perp \nabla((1, u_i)^T f(x_l)) - \nabla(c(x_l)) y_l \geq 0 \\
& \quad \forall l = 1, \ldots, q, \\
& \quad 0 \leq y_l \perp c(x_l) \geq 0 \quad \forall l = 1, \ldots, q,
\end{align*}$$

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 (6) and (8) are nonconvex optimization problems because of the presence of the complementarity constraints and the upper bound on $\eta \leq \|f(x_i) - f(x_k)\|_2^2$. 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 \( \eta \). Thus, the goal programming version becomes

\[
\begin{align*}
\text{maximize} & \quad \sum_{i=1}^{p} \eta_i \\
\text{subject to} & \quad \eta_i \leq (f_i(x_k) - f_i(x_j))^2 \\
& \quad \forall 0 \leq k, l \leq q, k \neq l \text{ and } \forall i = 1, \ldots, p, \\
& \quad 0 \leq x_i - \nabla((1, u_i)^T f(x_j)) - \nabla c(x_i)y_i \geq 0 \\
& \quad \forall l = 1, \ldots, q, \\
& \quad 0 \leq y_l - c(x_i) \geq 0 \\
& \quad 0 \leq u_l - \hat{f}(x_i) \leq z_l.
\end{align*}
\]

Similarly we can define componentwise versions with the first-order conditions of \( \text{SUM}(w) \). 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 \( \text{SUM}(w) \) and \( \text{GOAL}(z) \) characterize a Pareto point. This result is a direct corollary of Theorem 1.2.

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

1. \((x^*, y^*)\) solves the first-order conditions of \( \text{SUM}(w) \) for some weights \( w \geq 0 \) with \( e^T w = 1 \), or
2. \((x^*, y^*, u^*)\) solves the first-order conditions of \( \text{GOAL}(z) \) for some goals \( z \).

Clearly, the solution of the bilevel program (5) gives rise to a set of Pareto points.

**Proposition 2.2.** Let Assumptions A1–A4 hold. Then it follows that if

1. \((x_1^*, y_1^*, w_1^*, \eta^*)\) solves problem (6), then \((x_1^*, f_1^*)\) are Pareto points of \( \text{MOOP} \);
2. \((x_1^*, y_1^*, u_1^*, z_1^*, \eta^*)\) solves problem (8), then \((x_1^*, f_1^*)\) are Pareto points of \( \text{MOOP} \).

Moreover, in each case, if \( \eta^* \) is the global maximizer, then \( \eta^* \) 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) (Anitescu 2005, Fletcher et al. 2006). For example, a suitable NLP formulation of the MPCC (6) is given by

\[
\begin{align*}
\text{maximize} & \quad \eta \\
\text{subject to} & \quad \eta \leq \|f(x_k) - f(x_j)\|^2 \quad \forall 0 \leq k, l \leq q, k \neq l, \\
& \quad e^T w_l = 1 \quad \forall l = 1, \ldots, q, \\
& \quad s_l = \nabla (w_l T f(x_i)) - \nabla c(x_i)y_l \quad \forall l = 1, \ldots, q, \\
& \quad x_i \geq 0, \quad s_l \geq 0, \quad x_l^T s_l \leq 0 \quad \forall l = 1, \ldots, q, \\
& \quad t_l = c(x_i) \quad \forall l = 1, \ldots, q, \\
& \quad y_l \geq 0, \quad t_l \geq 0, \quad y_l^T t_l \leq 0 \quad \forall l = 1, \ldots, q,
\end{align*}
\]

where we have introduced slacks to obtain a numerically favorable formulation. It is well known that (10) violates the Mangasarian-Fromowitz constraint qualification at any feasible point (Chen and Florian 1995) 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, Fletcher et al. (2006) have shown that any stationary point of the NLP (10) is a strongly stationary point (Scheel and Scholtes 2000) of the MPCC (6) and vice versa. This fact has been used to show that standard NLP solvers can tackle MPCCs reliably and efficiently provided an MPCC-LICQ holds (Anitescu 2005, Benson et al. 2006, Fletcher et al. 2006, Fletcher and Leyffer 2004, Leyffer 2003, Leyffer et al. 2006, Liu et al. 2006, Raghunathan and Biegler 2005). We note that similar results hold for other nonlinear formulations of the complementarity conditions (Leyffer 2006).

Next, we analyze the complementarity constraints further. We prove that if the single-objective NLP satisfies the linear-independence constraint qualification and a second-order sufficient condition, then the constraint normals of the first-order conditions are linearly independent. We state this result in a slightly more general form.

**Proposition 2.3.** Consider the general single-objective nonlinear program

\[
\begin{align*}
\text{minimize} & \quad F(x) \quad \text{subject to} \quad G(x) \geq 0,
\end{align*}
\]

where \( F: \mathbb{R}^n \rightarrow \mathbb{R} \) and \( G: \mathbb{R}^n \rightarrow \mathbb{R}^m \) are twice continuously differentiable. Let \( x^* \) be a solution that satisfies the linear-independence constraint qualification and a second-order sufficient condition. Then it follows that the active constraint normals of the mixed complementarity problem corresponding to the first-order conditions of (11),

\[
\begin{align*}
\nabla F(x) + \nabla G(x)^T y &= 0, \\
0 &\leq y \perp G(x) \geq 0,
\end{align*}
\]

are linearly independent.
Let \((x^*, y^*)\) be the optimal primal-dual solution of (11). The active constraints are defined as
\[\bar{s} := \{i : G_i(x^*) = 0\}.
\]

We introduce the following notation,
\[A_s := [\nabla G_i^s]_{i \in \bar{s}}^T, \quad W_s := \nabla^2 F + \sum_{i=1}^m y_i^2 \nabla^2 G_i^s, \quad \text{and}
\]
\[I_s := [e_i]_{i \notin \bar{s}},
\]

to denote the various parts of the active constraint normals. To prove the result, we need to show that the basis matrix
\[
B_s := \begin{bmatrix} W_s & A_s \\ A_s^T & 0 \\ 0 & I_s \end{bmatrix}
\]
has linearly independent columns.

The proof is by contradiction, and we assume that there exists \(s = (s_x, s_y) \neq 0\) such that \(B_s s = 0\). The last two equations imply that \(s_y = 0\) and that \(A_s^T s_x = 0\), and we are left with \(W_s s_x = 0\). Premultiplying by \(s_x^T\) gives \(s_x^T W_s s_x = 0\), which contradicts the second-order sufficient condition, namely, that \(s_x^T W_s s_x > 0\) for all \(s_x \neq 0\) such that \(A_s^T s_x = 0\). Thus, the columns of \(B_s\) are linearly independent. \(\Box\)

Proposition 2.3 ensures that the complementarity constraints of (6) and (8) satisfy an MPCC-LICQ condition (Scheel and Scholtes 2000) whenever the underlying single-objective NLP satisfies an LICQ and a second-order sufficient condition. However, this result does not prove that the MPCC (6) or (8) satisfies an MPCC-LICQ, because degeneracy may exists in the constraints that define the maximum uniformity, \(\eta\).

One limitation of our approach is the fact that even linear MOOPs such as
\[
\begin{aligned}
\text{maximize} & \quad C^T x \\
\text{subject to} & \quad A^T x \geq b, \\
& \quad x \geq 0,
\end{aligned}
\]
lead to nonconvex NLP formulations. The reason for the nonconvexity of (6) is the presence of the constraints \(\eta \leq \|C^T x - C^T x^*\|^2\) and the presence of the complementarity constraints. Thus, in general, we cannot expect to find the global minimum of (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 be convex (Assumption A4). Consider the MOOP
\[
\begin{aligned}
\text{minimize}_{x} & \quad (x^2 - 1)^2, (x^2 - 4)^2.
\end{aligned}
\]
It follows that \(f_1(x) = (x^2 - 1)^2\) has two minimizers at \(x = \pm 1\) and a maximum at \(x = 0\). Likewise, \(f_2(x) = (x^2 - 4)^2\) has two minimizers at \(x = \pm 2\) and a maximum at \(x = 0\). However, the MPCC (6) cannot distinguish between minima and maxima. For this example, the MPCC approach generates the two “Pareto” points \(x_1 = 1\) and \(x_2 = 0\), which maximize the uniformity of representation. However, the second Pareto point, \(x_2 = 0\), clearly corresponds to a maximizer of the lower-level problem. Thus, for nonconvex MOOPs, the MPCC approach has a bias toward generating both minima and maxima of the MOOP, because such a choice of controls maximizes the separation between the objective values. Note that we could still use the bilevel formulation (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 http://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 (6) or (8). The failures were caused by the nonconvexity of the MPCC formulation, which can cause the NLP solvers to converge to a local minimum of the constraint violation.

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 (Dirkse and Ferris 1995, Ferris and Munson 2000). This is a standard strategy for solving complex MPCCs and is readily implemented in AMPL (Fourer et al. 2003) by using 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 (6) and (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. The results for the start-up with PATH and their computational cost are included in Table 3.

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 \(p\), the type of objectives and constraints, and whether or not the problem is convex (C) in the final column. We note that our collection contains the nonconvex problems ABC-comp, ex002, and ex004.
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 generates large sparse problems that are output in AMPL format. 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 with the NCP formulation is modest, while the increase in the number of constraints corresponds to the addition of the constraints $\eta \leq \cdots$, which is of order $q^2$. We also note that formulation (8) gives rise to the largest MPCCs because we have added multipliers of the goal constraints.

We note that the problem sizes differ for the NCP and MPCC formulations. The reason is that the NCP fixes the upper-level variables, $w_1$, to obtain a feasible solution. The differences between the MPCC formulations are due to the fact that in (7) we have fixed one weight from (6) to one. Moreover, (8) contains variables corresponding to the objective multipliers $u_1$, in addition to the goals $z_1$.

The problems are formulated in AMPL, and the initial NCPs are solved by using PATH. PATH implements a generalized Newton method that solves a linear complementarity problem to compute the search direction. The MPCCs are solved by using filterSQP (Fletcher and Leyffer 2002, 2004), which automatically reformulates the complementarity constraints as nonlinear equations. This solver implements a sequential quadratic programming algorithm with a filter to promote global convergence (Fletcher et al. 2002).

### Table 1: Multiobjective Optimization Problem Characteristics

<table>
<thead>
<tr>
<th>Name</th>
<th>$n$</th>
<th>$m$</th>
<th>$p$</th>
<th>Source</th>
<th>Objective</th>
<th>Constraints</th>
<th>$C$</th>
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<tr>
<td>ABC-comp</td>
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<td>3</td>
<td>2</td>
<td>Hwang and Masud (1979)</td>
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<td>Bilinear</td>
<td>Y</td>
</tr>
<tr>
<td>ex001</td>
<td>5</td>
<td>3</td>
<td>2</td>
<td>Das and Dennis (1997)</td>
<td>Quadratic</td>
<td>Quadratic</td>
<td>Y</td>
</tr>
<tr>
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<td>2</td>
<td>2</td>
<td>Wang and Renaud (1999)</td>
<td>Quadratic</td>
<td>Nonlinear</td>
<td>N</td>
</tr>
<tr>
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<td>2</td>
<td>2</td>
<td>Tappeta and Renaud (1999)</td>
<td>Quadratic</td>
<td>Nonlinear</td>
<td>N</td>
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<tr>
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<td>3</td>
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<td>Oliveira and Ferreira (2000)</td>
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<td>Linear</td>
<td>N</td>
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<tr>
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<td>Bounds</td>
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<td>Linear</td>
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<td>Steuer (1986)</td>
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### Table 2: Characteristics of NCP and MPCC Formulations

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<th>$n$</th>
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<td>420</td>
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which is clearly dominated by the lower point. Pareto point, namely, the point provides greater uniformity. We note, however, that the Pareto set with optimal weights, which clearly computed Pareto set for ex004. On the left is the weakly dominated Pareto points. Figure 3 shows the convex example ABC-comp. valid approximations of the Pareto set for the nonconvex MOOPs. Despite this shortcoming, we are able to find Kuhn-Tucker (KKT) conditions to characterize local maxima. The approach maybe even more robust if we allow ourselves to cycle through the objectives in turn.

We are interested in discovering how close the MPCC approach gets to the global maximum. Unfortunately, it would be prohibitive to run global optimization software on these test problems. Thus, we have conducted a small experiment by running the global optimization solver Baron (Tawarmalani and Sahinidis 2002, Sahinidis 2000) on the smallest MOOP, namely, the GOAL(\(z\)) formulation of ex005 for a reduced number of Pareto points (\(q = 8\)). Baron is a branch-and-reduce solver that generates valid bounds by constructing (local) outer approximations of the nonconvex functions that are refined in a branch-and-bound tree search. Even though Baron did not find the global maximum in 36,000 seconds CPU time, the

The results of MOLPg-\(q^*\) for NCP, (6), and (7) are also of interest. In these cases, the optimal uniformity is \(\eta^* = 0\), which corresponds to two or more coalescing Pareto points. Typically, however, the MPCC approaches are able to improve the uniformity by orders of magnitude compared with the uniform representation corresponding to NCP. In our experiments, (7) obtained better uniformity than (6) on two examples: ex003 and MOQP-01. We believe that there may be numerical reasons that make (7) preferable on some examples.

The results in Table 3 show that the MPCC formulation based on goal programming, (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. The better performance of the goal-programming-based approach (8) is not surprising, given its superior theoretical properties. We also note that in our experiments we arbitrarily fixed the first objective as the main objective in GOAL(\(z\)). The approach may be even more robust if we allow ourselves to cycle through the objectives in turn.

We are interested in discovering how close the MPCC approach gets to the global maximum. Unfortunately, it would be prohibitive to run global optimization software on these test problems. Thus, we have conducted a small experiment by running the global optimization solver Baron (Tawarmalani and Sahinidis 2002, Sahinidis 2000) on the smallest MOOP, namely, the GOAL(\(z\)) formulation of ex005 for a reduced number of Pareto points (\(q = 8\)). Baron is a branch-and-reduce solver that generates valid bounds by constructing (local) outer approximations of the nonconvex functions that are refined in a branch-and-bound tree search. Even though Baron did not find the global maximum in 36,000 seconds CPU time, the

### Table 3: Numerical Results for NCP and MPCC Formulations

<table>
<thead>
<tr>
<th>Name</th>
<th>Iteration</th>
<th>(\eta^*)</th>
<th>Iteration</th>
<th>(\eta^*)</th>
<th>Iteration</th>
<th>(\eta^*)</th>
<th>Iteration</th>
<th>(\eta^*)</th>
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<td>2.830E-1</td>
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<td>0</td>
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<td>0</td>
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<td>[I]</td>
<td>1,000</td>
<td>[I]</td>
<td>488</td>
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</tr>
</tbody>
</table>
results are still of interest. In particular, Baron gives the following valid bounds on the maximum: $0.3032 \leq \eta^* \leq 0.7055$. Table 4 gives the details of the runs, where we have added the results of the uniform distribution for comparison.

The approximate Pareto set for $q = 8$ is shown in Figure 4. The left plot shows the Pareto set of the NCP approach, which does not attempt to maximize uniformity. The plot on the right compares the Pareto sets obtained with the MPCC approach (crosses) and the global optimization solver Baron (circles). Surprisingly, the local MPCC solver finds a better solution than the global optimization approach. Of course, it is not clear whether even this solution is a global maximum, but the bounds obtained from Baron are encouraging. We note also that Baron finds its lower bound (candidate solution) after 2.54 seconds and spends the remainder of the time searching the tree for a better solution.

### 4. Conclusions and Outlook

We have presented a new approach to solving multi-objective optimization problems that approximates 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 present three 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. This is a nontrivial task, however, because AMPL would then have to provide derivatives up to third order for the Hessian matrices used in the NLP solvers.

Another limitation of our approach is the $\mathcal{O}(q^2)$ number of constraints that define the uniformity $\eta$ in (6) and (8). This limits the applicability of our approach to a mere 10 Pareto points. If more Pareto points were needed, then we could apply ideas similar to domain decomposition to partition the objective space, and then apply our approach to each partition.

Ultimately, we believe that our technique can be incorporated into interactive MOOP solution approaches such as www-nimbus (Miettinen and Mäkelä)
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.

Acknowledgments
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References


Miettinen, K., M. Mäkelä. 1998b. Theoretical and computational comparison of multiobjective optimization methods NIMBUS.


