# A Reduced Space Branch and Bound Algorithm for Global optimization 

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#### Abstract

A general class of branch and bound algorithms for solving a wide class of nonlinear programs with branching only in a subset of the problem variables is presented. By reducing the dimension of the search space, this technique may dramatically reduce the number of iterations and time required for convergence to $\epsilon$ tolerance while retaining proven exact convergence in the infinite limit. This presentation includes specifications of the class of nonlinear programs, a statement of a class of branch and bound algorithms, a convergence proof, and motivating examples with results.


Key words: Global optimization, branch and bound, reduced space, convex envelope

## 1. Introduction

One line of development of branch and bound algorithms involves solving a convex relaxation of the original problem to generate the lower bound. This approach stems from the work of Falk and Soland [4], Al-Khayyal and Falk [1], and McCormick $[10,11]$ where convex envelopes are used to replace nonconvex terms in developing the relaxation. Recent work in this line of development has focused on developing tighter constraints in the relaxation to produce higher lower bounds [2, 3, 18, 20, 21] or on reducing the variable domain [19] with the overall goal of reducing the need to branch. Branching is avoided because it involves the combinatorial search of a multidimensional space, and the computational work can grow exponentially. The reduced space algorithm presented below is intended to complement new or existing global optimization algorithms in this line of development by reducing the dimension of the search space for a wide class of problems.

Several other researchers have presented reduced space branch and bound algorithms, but these algorithms require problems with special properties. Phillips and Rosen [16] use branch and bound in a subset of the variable space in solving minimizations of a concave quadratic function over a bounded polyhedral set. Their algorithm branches only on the nonlinear variables, and it is able to solve problems with numerous linear variables. Horst and Thoai [7] presented a conical branch and bound algorithm for solving concave problems with numerous variables appearing linearly. The dimension of the problem to be solved via the branch and bound algorithm is only one dimension greater than the number of nonlinear vari-
ables. Muu and Oettli [13, 14] present a combined branch and bound and cutting plane algorithm to perform branch and bound in a subset of the problem variables. Their algorithm can treat problems with convex-concave constraints. Sherali and Alameddine [20] present a branch and bound algorithm based on the reformulationlinearization technique which has proven convergence for bilinear problems when branching on a subset of the variables. They point out that the algorithm can branch on the smaller of the two sets of variables. Horst and Thoai [8] present an algorithm for d.c. programming problems that branches in a reduced space. Phong, An, and Tao [17] present a reduced space branch and bound algorithm for indefinite quadratic programs which branches only on the concave variables.

The reduced space algorithm presented below is applicable to sparse nonlinear programs that can be expressed in factorable form, which includes most practical problems [11]. Smith and Pantelides [23] present an algorithm for reformulating expressions into the necessary form. Not all programs in factorable form will be able to branch in a reduced space, but any problem in factorable form can be quickly and automatically tested to see if it can use a reduced space.

The class of problems that can be solved in a reduced space is detailed in Section 1. Section 2 details the convex constraints that must be included in the convex relaxation used to obtain the lower bound. The reduced space algorithm is given in Section 3, and a convergence proof is provided in Section 4. Section 5 includes a comparison of full and reduced space solutions of three example problems, and Section 6 has some brief concluding remarks. The appendix contains a proposed algorithm for determining the minimal set of branching variables and details of the example problems.

## 2. Problem Definition

## Consider the problem,

Problem (P1)

$$
\begin{array}{cl}
\min _{x, y} & f(x, y) \\
\text { s.t. } & g(x, y) \leq 0 \\
& h(x, y) \leq 0 \\
& x \in X \\
& y \in Y \tag{5}
\end{array}
$$

with

$$
\begin{aligned}
& X:=[\underline{x}, \bar{x}] \subset R^{N}, Y:=[\underline{y}, \bar{y}] \subset R^{M} \\
& f: X \times Y \rightarrow R, g: X \times Y \rightarrow R^{G}, h: X \times Y \rightarrow R^{H} .
\end{aligned}
$$

Equality constraints may be included in this framework as a pair of opposing inequality constraints. In this formulation, the $y$ variables require branching, and
the $x$ variables do not. A proposed algorithm to determine $X$ and $Y$ for a program in factorable form is included in the appendix. To facilitate the presentation below, $D$ is introduced as the feasible space of problem P1,

$$
\begin{equation*}
D:=\{(x, y) \in X \times Y: g(x, y) \leq 0, h(x, y) \leq 0\} \tag{6}
\end{equation*}
$$

In order to guarantee convergence of the branch and bound algorithm while branching only in the $Y$ space, it is necessary to place some restrictions on the functions $f, g$, and $h . g$ must be a convex function, and $f$ and each element of $h$ must satisfy the conditions given below for function $w$. Let $w$ be any element of $h$ or $f$, so $w: X \times Y \rightarrow R$. Convergence can be established when $w$ has the following form:

$$
\begin{equation*}
w(x, y):=w^{A}(x)+\sum_{i \in Q} w_{i}^{B}(x) w_{i}^{C}(y)+w^{D}(y) \tag{7}
\end{equation*}
$$

where $Q$ is a set of indices indicating the bilinear interactions between functions of $x$ and functions of $y . w^{A}$ and $w^{B}$ must be convex, and $w^{C}$ and $w^{D}$ must be continuous. Further conditions on $w^{A}, w^{B}, w^{C}$, and $w^{D}$ are stated below after the necessary terminology has been defined.

It is assumed that $\underline{x}, \bar{x}, y$, and $\bar{y}$ are finite; thus, $X$ and $Y$ are compact sets that can be thought of as $N$ and $M$ dimensional rectangles. The partition sets used by this algorithm are all rectangular and compact with

$$
\begin{align*}
X^{k} & :=\left[\underline{x}^{k}, \bar{x}^{k}\right],  \tag{8}\\
Y^{k} & :=\left[\underline{y}^{k}, \bar{y}^{k}\right] . \tag{9}
\end{align*}
$$

Tuy [24] showed that rectangular subdivisions are weakly exhaustive. Some definitions are required for the presentation of the underestimating program, algorithm and proof.

DEFINITION 1. Given a set $X \times Y$, the subdivision of partition sets of $X \times Y$ is called exhaustive on $Y$, if it produces an infinite, nested sequence of partition sets, $\left\{\left(X^{k}, Y^{k}\right)\right\}$ and an associated sequence of diameters $d\left(Y^{k}\right)$ satisfying the following:

$$
\begin{align*}
\left(X^{0}, Y^{0}\right) & \supset\left(X^{1}, Y^{1}\right) \supset \cdots \supset\left(X^{k}, Y^{k}\right)  \tag{10}\\
\lim _{k \rightarrow \infty} d\left(Y^{k}\right) & =0  \tag{11}\\
\lim _{k \rightarrow \infty} Y^{k} & =\bigcap_{k} Y^{k}=\{\dot{y}\} . \tag{12}
\end{align*}
$$

This definition is an extension of Horst's [6] whose definition is recovered when $X$ is empty in which case the subdivision is just called exhaustive.

DEFINITION 2. A convex underestimator of a function $\varphi(y)$ over the domain $Y^{k}$ is a convex function denoted $\breve{\varphi}^{k}(y)$ satisfying

$$
\begin{equation*}
\breve{\varphi}^{k}(y) \leq \varphi(y) \quad \forall y \in Y^{k} \tag{13}
\end{equation*}
$$

DEFINITION 3. A concave overestimator of a function $\varphi(y)$ over the domain $Y^{k}$ is a concave function denoted $\hat{\varphi}^{k}(y)$ satisfying

$$
\begin{equation*}
\hat{\varphi}^{k}(y) \geq \varphi(y) \quad \forall y \in Y^{k} \tag{14}
\end{equation*}
$$

DEFINITION 4 . Given a sequence of partition sets $\left\{\left(X^{k}, Y^{k}\right)\right\}$ produced by a subdivision of $X \times Y$ that is exhaustive on $Y$ with $Y^{k} \underset{k \rightarrow \infty}{\longrightarrow}\{\dot{y}\}$, a corresponding sequence $\left\{y^{k}\right\}$ with $y^{k} \in Y^{k}$, and a corresponding sequence $\left\{x^{k}\right\}$ with $x^{k} \in X^{k}$ with $\left\{x^{k}\right\} \rightarrow \dot{x}$, a convex underestimator or concave overestimator is strongly consistent on Y if there exist subsequences $\left\{\left(X^{q}, Y^{q}\right)\right\},\left\{y^{q}\right\}$, and $\left\{x^{q}\right\}$ satisfying

$$
\begin{align*}
& \breve{\varphi}^{q}\left(x^{q}, y^{q}\right) \underset{q \rightarrow \infty}{\longrightarrow} \varphi(\dot{x}, \dot{y}) \quad \text { or }  \tag{15}\\
& \hat{\varphi}^{q}\left(x^{q}, y^{q}\right) \underset{q \rightarrow \infty}{\longrightarrow} \varphi(\dot{x}, \dot{y}) . \tag{16}
\end{align*}
$$

When $X$ is vacuous, a convex underestimator or concave overestimator is called simply strongly consistent.

DEFINITION 5. A function, $\varphi$, has tight bounds if one can provide upper and lower bounds, $\bar{\varphi}^{k}$ and $\underline{\varphi}^{k}$ respectively, for any subrectangle $Y^{k}$ of $Y$ such that for any infinite sequence, $\left\{Y^{k}\right\}$, produced by an exhaustive subdivision with $Y^{K} \rightarrow\{\dot{y}\}$,

$$
\begin{align*}
\underline{\varphi}^{k} & \leq \varphi(y) \leq \bar{\varphi}^{k} \quad \forall y \in Y^{k}  \tag{17}\\
\lim _{k \rightarrow \infty} \underline{\varphi}^{k} & =\lim _{k \rightarrow \infty} \bar{\varphi}^{k}=\varphi(\dot{y}) \tag{18}
\end{align*}
$$

A function, $\varphi$ has continuous tight bounds if $\bar{\varphi}^{k}$ and $\underline{\varphi}^{k}$ are continuous functions of $\underline{y}^{k}$ and $\bar{y}^{k}$.

Having defined these concepts and notation, the sufficient criteria for convergence of the algorithm is that $f$ and $h$ have convex underestimators that are strongly consistent on $Y$. Such convex underestimators are available when $w$ satisfies the following formal conditions:

## Conditions W

1. $w^{A}, w^{B}$ are convex
2. $w^{C}, w^{D}$ are continuous
3. strongly consistent, convex underestimators are available for $w^{C}$ and $w^{D}$
4. strongly consistent, concave overestimators are available for $w^{C}$ and $w^{D}$
5. $w^{B}, w^{C}, w^{D}$ have continuous tight bounds
6. For each $i \in Q$, at least one of the following two conditions must hold
(a) $w_{i}^{B}(x):=c^{i \mathrm{~T}} x$ for some constant $c^{i} \in R^{N}$
(b) $w_{i}^{C}(y) \geq 0$ for all $y \in Y$; hence, $\underline{w}_{i}^{C k} \geq 0$

The following examples demonstrate some of the breadth of this class of functions:

$$
\begin{aligned}
w(x, y) & :=x^{\mathrm{T}} x+y^{\mathrm{T}} B y \\
w(x, y) & :=x^{\mathrm{T}} x+x^{\mathrm{T}} A y+y^{\mathrm{T}} B y, \\
w(x, y) & :=c^{\mathrm{T}} x+\sum_{i} x_{i}^{2} \exp \left(y_{i}\right) .
\end{aligned}
$$

Given convex underestimators for $f$ and $h$, the following convex nonlinear program is used to provide lower bounds and to test the feasibility of a partition set.

Problem (P2)

$$
\begin{array}{cl}
\min _{x, y} & \breve{f}^{k}(x, y) \\
\text { s.t. } & g(x, y) \leq 0 \\
& \breve{h}^{k}(x, y) \leq 0 \\
& x \in X^{k} \\
& y \in Y^{k} \tag{23}
\end{array}
$$

Based on the definition of convex underestimators, every feasible point of P1 in the subdomain $X^{k} \times Y^{k}$ is feasible in P 2 ; and the objective of P 2 is less than or equal to that of P 1 for all points in $X^{k} \times Y^{k}$. Thus, P 2 provides a valid lower bound for the solution of P 1 over the partition set $X^{k}$ and $Y^{k}$. It should be noted that problem P2 contains only the necessary constraints to guarantee convergence of the algorithm. If available, one may add tighter bounding constraints to P 2 such as $[2,3,18]$ as long as the constraints given in P2 remain.

## 3. Convex Underestimators

In this section, convex underestimators for $f$ and $h$ satisfying conditions W will be provided and proven to be strongly consistent on $Y$. This proof establishes the sufficient conditions for the underestimating program to guarantee convergence of the algorithm given below for a wide class of problems.

A convex underestimator of (7) is:

$$
\begin{equation*}
\breve{w}^{k}(x, y):=w^{A}(x)+\breve{w}^{D k}(y)+\sum_{i \in Q} W_{i}^{k}(x, y) \tag{24}
\end{equation*}
$$

with

$$
W_{i}^{k}(x, y):=
$$

$$
\left\{\begin{array}{l}
\max \left\{\begin{array}{l}
\bar{w}_{i}^{B k} \breve{w}_{i}^{C k}(y)+w_{i}^{B}(x) \bar{w}_{i}^{C k}-\bar{w}_{i}^{B k} \bar{w}_{i}^{C k}, \\
\underline{w}_{i}^{B k} \breve{w}_{i}^{C k}(y)+w_{i}^{B}(x) \underline{w}_{i}^{C k}-\underline{w}_{i}^{B k} \underline{w}_{i}^{C k}
\end{array}\right\} \text { if } \underline{w}^{B k} \geq 0  \tag{25}\\
\max \left\{\begin{array}{l}
\bar{w}_{i}^{B k} \hat{w}_{i}^{C k}(y)+w_{i}^{B}(x) \bar{w}_{i}^{C k}-\bar{w}_{i}^{B k} \bar{w}_{i}^{C k}, \\
\underline{w}_{i}^{B k} \hat{w}_{i}^{C k}(y)+w_{i}^{B}(x) \underline{w}_{i}^{C k}-\underline{w}_{i}^{B k} \underline{w}_{i}^{C k}
\end{array}\right\} \text { if } \bar{w}^{B k}<0 \\
\max \left\{\begin{array}{l}
\bar{w}_{i}^{B k} \breve{w}_{i}^{C k}(y)+w_{i}^{B}(x) \bar{w}_{i}^{C k}-\bar{w}_{i}^{B k} \bar{w}_{i}^{C k}, \\
\underline{w}_{i}^{B k} \hat{w}_{i}^{C k}(y)+w_{i}^{B}(x) \underline{w}_{i}^{C k}-\underline{w}_{i}^{B k} \underline{w}_{i}^{C k}
\end{array}\right\} \text { otherwise }
\end{array}\right.
$$

The proof that (24) is a convex underestimator of $w$ follows from [10, 11], and these references also provide a method for providing the strongly consistent, convex underestimators and concave overestimators for the nonconvex functions of $y$. The convexity of (25) follows from the definitions of convex underestimators and convex overestimators, property 6 , and the fact that a maximum of two convex functions is convex. Each term of (24) is convex, so (24) is convex.
LEMMA 1. Given a function, $w$, in form (7) satisfying properties $1-6$, then $\breve{w}$ given by (24) is strongly consistent on $Y$.

Proof. The definition provides that there is a sequence of subrectangles $\left\{\left(X^{k}, Y^{k}\right)\right\}$ produced by a subdivision that is exhaustive on $Y$, a corresponding sequence $\left\{y^{k}\right\}$ with $y^{k} \in Y^{k}$, and a corresponding sequence $\left\{x^{k}\right\}$ with $x^{k} \in X^{k}$ and $x^{k} \rightarrow \dot{x}$. From the definition of an exhaustive subdivision, we have that $Y^{k} \rightarrow\{\dot{y}\}$, and it follows that $y^{k} \rightarrow \dot{y}$. The upper and lower bounds on $X^{k}$ are both sequences in a compact space, so there exists a convergent subsequence, so $X^{q} \rightarrow X^{*}=\left[\underline{x}^{*}, \bar{x}^{*}\right]$. Corresponding to this subsequence, there is the sequence $\left\{\left(\underline{x}^{q}, \bar{x}^{q}, \underline{y}^{q}, \bar{y}^{q}, y^{q}, x^{q}\right)\right\} \rightarrow\left(\underline{x}^{*}, \bar{x}^{*}, \dot{y}, \dot{y}, \dot{y}, \dot{x}\right)$. From properties $1-5, \breve{w}^{q}$ can be considered as a continuous function of $\left(\underline{x}^{q}, \bar{x}^{q}, \underline{y}^{q}, \bar{y}^{q}, y^{q}, x^{q}\right)$; therefore, the limit of $\breve{w}^{q}$ as $q \rightarrow \infty$ is just $\breve{w}^{q}$ evaluated at the limiting values.

By property 3

$$
\lim _{q \rightarrow \infty} \breve{w}^{q}\left(x^{q}, y^{q}\right)=w^{A}(\dot{x})+w^{D}(\dot{y})+\sum_{i \in Q} W_{i}^{\infty}(\dot{x}, \dot{y})
$$

and applying properties 3 and 4 to $W_{i}^{\infty}$, equation (25) above with the limiting values inserted.

$$
W_{i}^{\infty}(\dot{x}, \dot{y})=w_{i}^{B}(\dot{x}) w_{i}^{C}(\dot{y})
$$

which completes the requirements for a strongly consistent convex underestimator.

## 4. Algorithm

This description of a general class of branch and bound algorithms is based largely on the ideas of previous researchers $[6,11,18,19]$. Here we present a general purpose branch and bound algorithm that includes branching on a subset of the variable
domain explicitly. Steps marked as optional can be left out without effecting the convergence proof that follows; in practice, they are helpful for some problems. Let $\beta\left(M^{k}\right)$ or $\beta\left(X^{k}, Y^{k}\right)$ refer to the optimal objective function value of P 2 for the region $M^{k}=\left(X^{k}, Y^{k}\right)$ and $z\left(M^{k}\right)$ or $z\left(X^{k}, Y^{k}\right)$ refer to an element of the corresponding argmin.

ALGORITHM 1. Reduced space branch and bound algorithm

## Initialization (iteration 0)

Step 1. Apply any finite methods to reduce the initial variable domain size without removing a global optimum (e.g. see the preprocessing step [18]) to produce $X^{0} \subseteq X$ and $Y^{0} \subseteq Y$. (optional)
Step 2. Solve problem P2, $\beta_{0}:=\beta\left(X^{0}, Y^{0}\right)$, and $z^{0}:=z\left(X^{0}, Y^{0}\right)$. If problem P 2 is infeasible, stop; problem P1 is infeasible.
Step 3. Apply finite variable domain reduction techniques guaranteed not to remove a global optimum [19, 22] to produce $X^{0 \prime} \subseteq X^{0}$ and $Y^{0 \prime} \subseteq Y^{0}$. If $X^{0 \prime} \neq X^{0}$ or $Y^{0 \prime} \neq Y^{0}$ and the limit to the number of variable domain reductions has not run out, $X^{0}:=X^{0 \prime}$ and $Y^{0}:=Y^{0 \prime}$ repeat step 3; otherwise, $X^{0}:=X^{0 \prime}$ and $Y^{0}:=Y^{0 \prime}$. (optional)
Step 4. Initialize the iteration counter $k:=1$, the partition $\underline{M}_{0}:=\left\{\left(X^{0}, Y^{0}\right)\right\}$, the upper bound $\alpha_{0}:=\infty$, and the set of feasible points $F^{0}:=\emptyset$.

Main Loop (iterations 1, 2, ...)
Step 5. Apply some finite method to search for feasible points (potential optima) of P 1 such as applying a local NLP solver to P 1 . Let $F$ be the potentially empty set of feasible points located by this procedure, assign $F^{k}:=$ $F \cup F^{k-1}$. This step need not be applied at every iteration of the main loop once a feasible point has been found. If it is skipped, $F^{k}:=F^{k-1}$.

$$
\begin{equation*}
\alpha_{k}:=\min _{z \in F^{k}} f(z) \tag{26}
\end{equation*}
$$

If $F^{k} \neq \emptyset$, define the best known feasible point

$$
\begin{equation*}
b^{k}:=\underset{z \in F^{k}}{\operatorname{argmin}} f(z) . \tag{27}
\end{equation*}
$$

Step 6. Remove elements of the current partition that cannot contain a solution

$$
\underline{R}_{k}:=\left\{M \in \underline{M}_{k-1}: \beta(M)<\alpha_{k}\right\} .
$$

Step 7. Choose a nonempty collection $P_{k} \subseteq \underline{R}_{k}$, and partition each element of $P_{k}$ into subrectangles only branching in the $Y$ space. Call the new partition sets $P_{k}^{\prime}$.

Step 8. For each $P \in P_{k}^{\prime}$ perform the following steps:

1. Apply finite variable domain reduction techniques guaranteed not to remove a global optimum [19] to produce $P^{*} \subseteq P$. Replace $P \in P_{k}^{\prime}$ with $P^{*}$, and $P:=P^{*}$. (optional)
2. Solve P 2 to obtain $\beta(P)$, if P 2 is infeasible or $\beta(P)>\alpha_{k}$ remove $P$ from $P_{k}^{\prime}$ and skip to next element of $P_{k}^{\prime}$.
3. Apply finite variable domain reduction techniques guaranteed not to remove a global optimum [19] to produce $P^{*} \subseteq P$. Replace $P \in P_{k}^{\prime}$ with $P^{*}$. (optional)
4. If the number of variable domain reductions allowed has not run out and $P^{*} \neq P$, set $P:=P^{*}$ and return to step 2. (optional)
Step 9. The partition set remaining is now

$$
\begin{equation*}
\underline{M}_{k}:=\left(\underline{R}_{k} \backslash P_{k}\right) \cup P_{k}^{\prime} \tag{28}
\end{equation*}
$$

giving a new lower bound of

$$
\begin{equation*}
\beta_{k}:=\inf _{M \in \underline{M}_{k}} \beta(M) \tag{29}
\end{equation*}
$$

If $\underline{M}_{k}$ is empty, $\beta_{k}=\infty$. For the sake of the convergence proof, if $\underline{M}_{k} \neq \emptyset$ the following definitions apply

$$
\begin{align*}
M_{k} & \in \underset{M \in \underline{M}_{k}}{\operatorname{argmin}} \beta(M),  \tag{30}\\
z^{k} & :=z\left(M_{k}\right) . \tag{31}
\end{align*}
$$

Step 10. If $\alpha_{k}-\beta_{k}>0(\geq \epsilon), k:=k+1$ and return to step 5; otherwise, the problem is solved. If $F^{k}=\emptyset$, the problem is infeasible; otherwise, $\alpha_{k}=\beta_{k}$ is the solution of P 1 , and $b^{k}$ is an optimal solution.
This algorithm includes the possibility of reducing the domain of the $x$ variables, but it is not required for convergence. If the variable domain reduction techniques are not used, $X^{0}=X^{1}=X^{2} \cdots$.

## 5. Convergence Proof

Let $Z^{a}$ be the set of accumulation points of $z^{k}$, and let $Z^{*}$ be the $\operatorname{argmin}_{(x, y) \in D} f(x, y)$.
THEOREM 1. If a reduced space branch and bound algorithm satisfying the following conditions

1. the subdivision of partition sets in step 7 is exhaustive on $Y$
2. the selection of elements to be partitioned in step 7 is bound improving
3. the convex subfunctionals, $\breve{f}$ and $\breve{h}$, used in problem $P 2$ are strongly consistent on $Y$
is applied to problems in the form P1 with $D \neq \emptyset$, then an infinite application of the algorithm will produce
4. $\beta:=\lim _{k \rightarrow \infty} \beta_{k}=\min _{(x, y) \in D} f(x, y)$
5. $Z^{a} \subset Z^{*}$

Proof. For every iteration, $k=0,1,2, \ldots$, of the algorithm, by design the following is true

$$
\begin{align*}
\beta_{k} & \leq \min _{(x, y) \in D} f(x, y),  \tag{32}\\
M_{k} & \in \underset{M \in \underline{M}_{k}}{\operatorname{argmin}} \beta(M),  \tag{33}\\
\left(x^{k}, y^{k}\right) & =z^{k} \in z\left(M_{k}\right) . \tag{34}
\end{align*}
$$

Horst [6] gives that $\left\{\beta_{k}\right\}$ is a nondecreasing sequence bounded above by $\min _{(x, y) \in D}$ $f(x, y)$, which guarantees the existence of the limit

$$
\begin{equation*}
\beta:=\lim _{k \rightarrow \infty} \beta_{k} \leq \min _{(x, y) \in D} f(x, y) . \tag{35}
\end{equation*}
$$

$\left\{z^{k}\right\}$ is a sequence on a compact set, therefore, it has a convergent subsequence. For any $(\breve{x}, \breve{y})=\check{z} \in Z^{a}$, there exists a subsequence $\left\{z^{r}\right\}$ of $\left\{z^{k}\right\}$ with

$$
\begin{equation*}
\lim _{r \rightarrow \infty} z^{r}=\check{z} \tag{36}
\end{equation*}
$$

From properties 1 and 2, we have based on previous work [5], there exists a decreasing subsequence $Y_{q} \subset Y_{r}$ where $Y_{r}$ is the $Y$ space of the partition $M_{r}$ with

$$
\begin{align*}
y^{q} & \in Y_{q},  \tag{37}\\
\left(x^{q}, y^{q}\right) & \in M_{q},  \tag{38}\\
\beta_{q} & =\beta\left(M_{q}\right)=\breve{f}^{q}\left(x^{q}, y^{q}\right),  \tag{39}\\
\lim _{q \rightarrow \infty} y^{q} & =\{\check{y}\} . \tag{40}
\end{align*}
$$

By property 3, it follows that

$$
\begin{equation*}
\lim _{q \rightarrow \infty} \beta_{q}=\beta=f(\check{x}, \check{y}) \tag{41}
\end{equation*}
$$

All that remains is to prove that $(\check{x}, \check{y}) \in D . X$ and $Y$ are closed sets, so $(\check{x}, \check{y}) \in$ $X \times Y$. The remainder of the proof will be by contradiction.

Assume $(\check{x}, \breve{y}) \notin D$, then

$$
\begin{equation*}
\max \left\{\max _{i} g_{i}(\check{x}, \check{y}), \max _{j} h_{j}(\check{x}, \check{y})\right\}=\delta>0 \tag{42}
\end{equation*}
$$

There are two cases, either $g_{i}(\check{x}, \check{y})=\delta>0$ for some $i$ or $h_{j}(\check{x}, \check{y})=\delta>0$ for some $j$. Consider the first case, $g_{i}$ is convex and hence continuous; therefore, the sequence $\left\{g_{i}\left(x^{q}, y^{q}\right)\right\}$ converges to $g_{i}(\check{x}, \check{y})$. By definition of convergence,
$\exists q_{\delta}$ such that $q>q_{\delta} \rightarrow\left|g_{i}\left(x^{q}, y^{q}\right)-g_{i}(\check{x}, \check{y})\right|<\delta$. Therefore for $q>q_{\delta}$, $g_{i}\left(x^{q}, y^{q}\right)>0$ implying that P2 is infeasible and violating the assumption that $\left(x^{q}, y^{q}\right)=z^{q}=z\left(M_{q}\right)$.

The second case is that $h_{j}(\check{x}, \check{y})=\delta>0$ for some $j$. From the property 3 , the sequence $\left\{\breve{h}_{j}^{q}\left(x^{q}, y^{q}\right)\right\}$ converges to $h_{j}(\breve{x}, \check{y})$. By a similar argument, $\exists q_{\delta}$ such that $q>q_{\delta} \rightarrow \breve{h}_{j}^{q}\left(x^{q}, y^{q}\right)>0$ implying that P 2 is infeasible. Both cases result in a contradiction, therefore $(\breve{x}, \breve{y}) \in D$.

$$
\begin{gather*}
\beta=f(\check{x}, \check{y})=\min _{(x, y) \in D} f(x, y)  \tag{43}\\
(\breve{x}, \check{y}) \in Z^{*} \tag{44}
\end{gather*}
$$

## 6. Examples

We have chosen three examples to illustrate the breadth of problems to which the reduced space algorithm may be applied and to demonstrate how branching in the reduced space can dramatically decrease the runtime and number of iterations required to converge to a given tolerance. In each example, the dimension of $y$ is much less than the dimension of $x$, which is the case where this approach is most effective. Before the examples and results are presented, we provide a description of our test program.

### 6.1. ImPLEMENTATION DETAILS

Branching in the reduced space can be used with any algorithm satisfying the general description provided above. For the sake of testing, we implemented a branch and bound algorithm in $\mathrm{C}++$ on a 50 MHz Sun SPARC 10 . The program reads in a problem description file, automatically determines the minimal set of variables that require branching using the proposed algorithm in the appendix, solves the problem, and outputs the results. When testing with full space branching, the second step is skipped; all other aspects of the algorithm are kept constant between the two modes.

There are many important details that go into the implementation of an algorithm of the form given above. Only the most crucial aspects of the algorithm will be described here. Optional steps 1,3 and 8.1 are omitted, and the number of variable domain reductions per main loop iteration in step 8.3 is limited to four.

The LP and/or NLP subproblems generated by the program in steps 5 and 8.2 use the convex/concave envelopes as presented by McCormick [11] to provide the lower bounding relaxations, and they are solved with direct calls to MINOS 5.5 [12] using warm or hot starts when possible. In step 5, MINOS 5.5 is applied to the original problem P1 to search for local minima. The program solves P1 each main loop iteration until it finds a local minimum, and afterwards, it solves P1 with
decreasing frequency. The underestimating program solved in step 8.2 is equivalent to P2; no additional constraints are used. In step 8.3, active variable bounds are used to reduce the variable domain according to the methods of Ryoo and Sahinidis [19].

The last crucial detail of the implementation is the splitting strategy employed. In step 7, the region with the least lower bound is split into two subrectangles. The splitting process works in two steps: choosing which variable to split on and choosing where to split. Before entering step 7, the program solved the relaxation P2 for the region to be split. The relaxation provides a point and estimates of the nonconvex terms. The variable is chosen to maximize the difference between the estimate of a nonconvex term and the actual value of the nonconvex term at the relaxation solution. The choice of variable is restricted to the reduced space unless the full space option is requested.

Assume that $i$ is the index of the chosen variable. If $F^{k}$, the set of known feasible points, is not empty, $b^{k}$ is the best known feasible solution. $y^{k}$ is the solution of the relaxed problem if available. Here is the algorithm used to determine the split location:

ALGORITHM 2. Method for choosing a split location
IF $\left(F^{k} \neq \emptyset\right)$ THEN
$\operatorname{IF}\left(b_{i}^{k} \in \operatorname{interior}\left(\left[\underline{y}_{i}^{k}+\epsilon^{0.6}, \bar{y}_{i}^{k}-\epsilon^{0.6}\right]\right)\right.$ ) THEN Split at $b_{i}^{k}$
ELSE

$$
\text { lowerCloser : }=\left|b_{i}^{k}-\underline{y}_{i}^{k}\right| \leq\left|b_{i}^{k}-\bar{y}_{i}^{k}\right|
$$

IF (No Relaxed Solution) THEN IF (lowerCloser) THEN Split at $0.1 \bar{y}_{i}^{k}+0.9 \underline{y}_{i}^{k}$

$$
\text { ELSE Split at } 0.9 \bar{y}_{i}^{k}+0.1 \underline{y}_{i}^{k}
$$

## ELSE

IF (lowerCloser) THEN

$$
y_{i}^{k}:=\max \left\{y_{i}^{k}, \underline{y}_{i}^{k}+0.01\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\}
$$

$$
y_{i}^{k}:=\min \left\{y_{i}^{k}, \bar{y}_{i}^{k}-0.05\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\}
$$

## ELSE

$$
\begin{aligned}
y_{i}^{k} & =\max \left\{y_{i}^{k}, y_{i}^{k}+0.05\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\} \\
y_{i}^{k} & :=\min \left\{y_{i}^{k}, \bar{y}_{i}^{k}-0.01\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\}
\end{aligned}
$$

## END

## Split at $y_{i}^{k}$

## END

END
ELSE
IF (No Relaxed Solution) THEN

$$
\text { Split at }\left(\underline{y}_{i}^{k}+\bar{y}_{i}^{k}\right) / 2
$$

ELSE

$$
y_{i}^{k}:=\max \left\{y_{i}^{k}, \underline{y}_{i}^{k}+0.05\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\}
$$

```
    \(y_{i}^{k}:=\min \left\{y_{i}^{k}, \bar{y}_{i}^{k}-0.05\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)\right\}\)
    Split at \(y_{i}^{k}\)
    END
END
```

$\epsilon$ is small positive number which indicates machine precision. This splitting procedure guarantees that the width of the intervals produced are bounded above by either $\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}-\epsilon^{0.6}\right.$ ) (case i) or by $0.99\left(\bar{y}_{i}^{k}-\underline{y}_{i}^{k}\right)$ (case ii). In an infinite application of branching procedure to variable $i$, case i can only apply a finite number of times. Let $j$ be the index of the last time that case i applied. For all remaining elements in the infinite sequence, $0 \leq \bar{y}_{i}^{l}-\underline{y}_{i}^{l} \leq 0.99^{l-j}\left(\bar{y}_{i}^{j}-\underline{y}_{i}^{j}\right)$. $\lim _{l \rightarrow \infty}\left(\bar{y}_{i}^{l}-\underline{y}_{i}^{l}\right)=0$.

A relative tolerance of 0.0001 was used as the termination criteria for all the examples. The algorithm also terminates if a time limit of 100000 CPU seconds or an iteration of 1000000 is exceeded. The first two examples were solved to tolerance using both full and reduced space modes, and the last example was solved to tolerance only in the reduced space mode.

### 6.2. BILINEAR EXAMPLE

This randomly generated problem has a linear objective function, ten linear constraints and twenty bilinear constraints. It has twenty-three variables of which only three need branching with the reduced space algorithm.

$$
\begin{array}{ll}
\min _{x, y} & c^{\mathrm{T}}\left[\begin{array}{l}
x \\
y
\end{array}\right] \\
\text { s.t. } & A\left[\begin{array}{l}
x \\
y
\end{array}\right] \leq b \\
& \sum_{i=1}^{20} \sum_{j=1}^{3} B_{k i j} x_{i} y_{j} \leq d_{k} ; k=1, \ldots, 20 \\
& -2 \leq y_{j} \leq 2 ; j=1, \ldots, 3 \\
& -2 \leq x_{i} \leq 2 ; i=1, \ldots, 20 \tag{49}
\end{array}
$$

with

$$
\begin{aligned}
& c \in R^{23} \\
& A \in R^{10 \times 23} \\
& B \in R^{20 \times 20 \times 3}
\end{aligned}
$$

Tables IV, V, VI, and VII, appearing in the appendix, provide the nonzero elements of $c, d, A$, and $B$ respectively.

The algorithm statistics comparing the reduced space and full space modes are shown in Table I. Both versions of the algorithm locate the same global minimum
in an acceptable amount of time; however, the reduced space version uses much fewer iterations and much less CPU time. In the process of solving this problem, three local minima were located by MINOS of which two are not global minima. The objective function values of these local minima are $-15.2843,-17.6430$, and -20.8008 . The number of relaxed problems is higher than the number of branch and bound iterations because the relaxed problem is resolved with a hot start after a variable domain reduction. The full space algorithm requires approximately eight times the CPU time and five times the number of iterations required by the reduced space algorithm.

Table I. Algorithm statistics for example one

| Space | Iterations | CPU <br> time (s) | Relaxations <br> solved | Original NLPs <br> solved |
| :--- | ---: | ---: | :---: | :---: |
| Reduced | 995 | 184.9 | 1472 | 34 |
| Full | 5157 | 1415.3 | 5961 | 79 |

### 6.3. PRoducts of convex and linear functions

The second example involves minimizing a convex objective function subject to constraints involving products of convex and linear functions. It is a small and simplified version of the formulation for batch reactor design under uncertainty developed by Ierapetritou and Pistikopoulos [9]. The problem has thirty-seven variables of which only two need branching with the reduced space algorithm. There are six linear constraints and sixteen nonconvex constraints. The problem has at least one non-global local minimum.

$$
\begin{array}{ll}
\min _{x, y} & \sum_{j=1}^{3} 3 \exp \left(0.6 x_{j}\right)+c^{\mathrm{T}}\left[\begin{array}{l}
x \\
y
\end{array}\right] \\
\text { s.t. } & x_{j}-y_{i} \geq \log \left(S_{i j}\right) ; i=\{1,2\}, j=\{1,2,3\} \\
& \sum_{i=1}^{2} x_{(3+2 j+i)} \exp \left(t_{i}-y_{i}\right) \leq 8 ; j=\{0, \ldots, 15\} \\
& \underline{x} \leq x \leq \bar{x} \\
& \underline{y} \leq y \leq \bar{y} \tag{54}
\end{array}
$$

with

$$
\begin{align*}
& S=\left[\begin{array}{lll}
2 & 3 & 4 \\
4 & 6 & 3
\end{array}\right]  \tag{55}\\
& t=\left[\begin{array}{l}
2.995732273553991 \\
2.772588722239781
\end{array}\right] \tag{56}
\end{align*}
$$

The variable bounds and objective function coefficients are presented in Table VIII.

Both versions find the same solution to this example, but the difference in time required for solution between the two versions is larger than example one. Table II shows the statistics for the two algorithms. The reduced space algorithm is faster than the full space algorithm by two orders of magnitude in CPU time, and it requires three orders of magnitude less iterations than the full space algorithm.

Table II. Algorithm statistics for example two

| Space | Iterations | CPU <br> time (s) | Relaxations <br> solved | Original NLPs <br> solved |
| :--- | ---: | ---: | :---: | :---: |
| Reduced | 25 | 9.87 | 31 | 5 |
| Full | 30789 | 6489.23 | 54174 | 176 |

### 6.4. Products of nonconvex and convex functions

The third example problem has a linear objective function, one linear constraint, and one nonconvex constraint involving the products of nonconvex, cubic functions and convex quadratic functions. The objective function coefficients for $x$ were randomly determined, and the objective function coefficients for $y$ were chosen. The constraints were chosen to give a nontrivial problem involving products of nonconvex and convex functions. The problem has twenty-three variables of which three require branching in the reduced space algorithm, and it has at least two nonglobal local minima.

$$
\begin{array}{ll}
\min _{x, y} & c^{\mathrm{T}}\left[\begin{array}{l}
y \\
x
\end{array}\right] \\
\text { s.t. } & \sum_{i=1}^{8}\left(0.1 y_{1}^{3}-0.2 y_{1}^{2}+0.01 y_{1}+10\right) 0.5 x_{i}^{2}+ \\
& \sum_{i=9}^{16}\left(0.1 y_{2}^{3}-0.2 y_{2}^{2}+0.01 y_{2}+10\right) 0.5 x_{i}^{2}+ \\
& \sum_{i=16}^{20}\left(0.1 y_{3}^{3}-0.2 y_{3}^{2}+0.01 y_{3}+10\right) 0.5 x_{i}^{2} \leq 250 \\
& y_{1}+y_{2}+y_{3}=0.5 \\
& -2 \leq y_{i} \leq 2 ; i=\{1,2,3\} \\
& 0 \leq x_{i} \leq 10 ; i=\{1, \ldots, 20\} \tag{61}
\end{array}
$$

The objective function coefficients appear in Table IX contained in the appendix.
The reduced space algorithm was able to find the global minimum to the specified tolerance within an acceptable amount of time, but the full space algorithm
exceeded the CPU time limit of 100000 CPU seconds. Table III shows the iterations required for the reduced space algorithm to converge to the specified tolerance, and for the full space algorithm, it shows the tolerance achieved within the CPU time limit. The reduced space algorithm requires only 4.664 CPU minutes, and the full space algorithm used over 27.77 CPU hours without converging.

Table III. Algorithm statistics for example three

| Space | Iterations | CPU <br> time (s) | Relaxations <br> solved | Original NLPs <br> solved | Tolerance |
| :--- | ---: | :---: | :---: | :---: | :---: |
| Reduced | 433 | 280 | 529 | 21 | $1.0 \times 10^{-4}$ |
| Full | 127328 | 100000 | 130730 | 462 | $2.3 \times 10^{-3}$ |

## 7. Conclusions

These examples demonstrate that the reduced space branch and bound algorithm can provide a dramatic reduction in the CPU time required to solve problems to finite tolerance when $N \gg M$, and the proofs given provide for exact convergence in the infinite limit. The examples also demonstrate some of the breadth of problems to which this technique can be applied.

Branching in a reduced space can be incorporated easily into existing branch and bound algorithms. The variables can be partitioned automatically or manually into subsets $x$ and $y$, and existing programs can use them by forbidding branches on variables in $x$.

## Appendix

## A. Automatic partitioning of variables

In this appendix, a proposed algorithm is presented to automatically determine the minimum set of variables, $Y$, that require branching for problems presented in the following factorable form:

$$
\begin{align*}
z_{j} & =x_{j} ; j=1, \ldots, n  \tag{62}\\
z_{j} & =\sum_{i=1}^{j-1}\left(c_{i}^{j} z_{i}+\xi_{i}^{j}\left(z_{i}\right)+\sum_{k=1}^{j-1} B_{i k}^{j} z_{i} z_{k}\right) ; j=n+1, \ldots, N \tag{63}
\end{align*}
$$

Some of the elements of $z$ are just intermediate variables added to put the problem in factorable form, but others are function values that are constrained by some lower or upper bound, $z^{L}$ or $z^{U}$ respectively. If $z_{j}$ is an intermediate value, $z_{j}^{L}=-\infty$ and $z_{j}^{U}=\infty$; otherwise, at least one of the bounds is finite. In a sparse problem, most of the elements of each $c^{j}$ and $B^{j}$ are zero, and many of the functions $\xi_{i}^{j}(\cdot)$ are functions whose value is always zero.

Let $I_{j}$ be the set of variables incident on the expression for $z_{j}$.

$$
I_{j}:=\left\{i \in 1, \ldots, j-1: c_{i}^{j} \neq 0\left|\xi_{i}^{j}(\cdot) \neq 0\right| \exists k \text { with }\left(B_{i k}^{j} \neq 0 \mid B_{k i}^{j} \neq 0\right)\right\}
$$

It is also useful to define the $\operatorname{Base} \operatorname{Vars}(j)$ function that determines the set of original variables on which the value of $z_{j}$ depends.

$$
\operatorname{BaseVars}(j):= \begin{cases}\left\{x_{j}\right\} & \text { for } j \leq n  \tag{64}\\ \bigcup_{i \in I_{j}} \operatorname{BaseVars}(i) & \text { otherwise }\end{cases}
$$

The assumptions of this work provide that all original variables have finite lower and upper bounds, $\underline{x}$ and $\bar{x}$ respectively. Lower and upper bounds for $z, \underline{z}$ and $\bar{z}$ respectively, are determined using existing interval mathematics techniques [15]. In addition to being able to provide bounds for $z$, it must be possible to determine whether each of the single variable functions $\xi$ is convex, concave, both, or neither over a specified domain. Let the following functions return a boolean value indicating whether the function has the indicated curvature over the domain $\left[\underline{z}_{i}, \bar{z}_{i}\right]$.

$$
\begin{align*}
& \text { Concave }\left(\xi_{i}^{j}, \underline{z}_{i}, \bar{z}_{i}\right):=\left\{\begin{array}{l}
\text { TRUE if } \xi_{i}^{j} \text { is concave on }\left[\underline{z}_{i}, \bar{z}_{i}\right] \\
\text { FALSE otherwise }
\end{array}\right.  \tag{65}\\
& \text { Convex }\left(\xi_{i}^{j}, \underline{z}_{i}, \bar{z}_{i}\right):=\left\{\begin{array}{l}
\text { TRUE if } \xi_{i}^{j} \text { is convex on }\left[\underline{z}_{i}, \bar{z}_{i}\right] \\
\text { FALSE otherwise }
\end{array}\right. \tag{66}
\end{align*}
$$

The algorithm is presented as three subroutines and a main driver. The purpose of the first two subroutines is to check a particular line of the formulation for the indicated curvature and to add variables to $Y$ to guarantee that the specified envelope becomes tight in the infinite limit. These subroutines also accumulate the set of bilinear interactions in $A$. Each element of $A$ is an ordered pair of nonempty sets $(L, R)$ where $L$ is the set of variables appearing on the left hand side of a multiplication and $R$ is the set of variables appearing on the right hand side. The third subroutine is used to choose which side of a bilinearity should be added to $Y$. These subroutines are directed by the main driver.

ALGORITHM 3. Subroutine to ensure a tight convex envelope
This subroutine examines the expression for $z_{j}$. It adds variables to $Y$ that are necessary for $z_{j}$ to have a tight convex envelope in the infinite limit, and it records the bilinear interactions between variables set $A$.

RequireConvex(integer $j$ )
IF $(j>n)$ THEN
FOR $i:=1$ TO $j-1$ BEGIN

```
    IF \(\left(c_{i}^{j}>0\right)\) RequireConvex \((i)\)
    IF \(\left(c_{i}^{j}<0\right)\) RequireConcave \((i)\)
    IF \(\left(\neg \operatorname{Convex}\left(\xi_{i}^{j}, \underline{z}_{i}, \bar{z}_{i}\right)\right) Y:=Y \cup \operatorname{BaseVars}\left(z_{i}\right)\)
    ELSE RequireConvex \((i)\)
    IF \(\left(B_{i i}^{j}>0\right)\) RequireConvex \((i)\)
    \(\operatorname{IF}\left(B_{i i}^{j}<0\right) Y:=Y \cup \operatorname{BaseVars}\left(z_{i}\right)\)
    FOR \(k:=1\) TO \(j-1\) BEGIN
        IF \(\left(i \neq k \wedge B_{i k}^{j} \neq 0\right)\) THEN
        \(A:=A \cup(\operatorname{BaseVars}(i), \operatorname{BaseVars}(k))\)
        \(Y:=Y \cup(\operatorname{BaseVars}(i) \cap \operatorname{BaseVars}(k))\)
        IF \(\left(B_{i k}^{j}>0\right)\) THEN
            IF \(\left(\bar{z}_{k}>0\right)\) RequireConvex \((i)\)
            IF \(\left(\underline{z}_{k}<0\right)\) RequireConcave \((i)\)
            IF \(\left(\bar{z}_{i}>0\right)\) RequireConvex \((k)\)
            IF \(\left(\underline{z}_{i}<0\right)\) RequireConcave \((k)\)
        ELSE
            IF \(\left(\bar{z}_{k}>0\right)\) RequireConcave \((i)\)
            IF \(\left(\underline{z}_{k}<0\right)\) RequireConvex \((i)\)
            IF ( \(\bar{z}_{i}>0\) ) RequireConcave \((k)\)
            IF \(\left(\underline{z}_{i}<0\right)\) RequireConvex \((k)\)
            END
        END
    END
    END
END
```

ALGORITHM 4. Subroutine to ensure a tight concave envelope
This is the analogous subroutine for ensuring a tight concave envelope.

```
RequireConcave(integer j)
IF (j>n) THEN
    FOR i:= 1 TO j-1 BEGIN
    IF (cij}>>0) RequireConcave(i
    IF ( cci
    IF (\negConcave ( }\mp@subsup{\xi}{i}{j},\mp@subsup{\underline{z}}{i}{},\mp@subsup{\overline{z}}{i}{\prime}))Y:=Y\cup\operatorname{BaseVars}(\mp@subsup{z}{i}{}
    ELSE RequireConcave(i)
    IF ( }\mp@subsup{B}{ii}{j}>0)Y:=Y\cup\operatorname{BaseVars}(\mp@subsup{z}{i}{}
    IF ( }\mp@subsup{B}{ii}{j}<0)\mathrm{ RequireConcave( }i\mathrm{ )
    FOR k:=1 TO j-1 BEGIN
        IF (i\not=k\wedge B}\mp@subsup{i}{ik}{j}\not=0) THE
            A:=A\cup(BaseVars(i), BaseVars(k))
```

```
        Y:=Y\cup(BaseVars}(i)\cap\operatorname{BaseVars}(k)
        IF ( }\mp@subsup{B}{ik}{j}<0) THE
            IF (玆}>>0)\mathrm{ RequireConvex(i)
            IF (\mp@subsup{\underline{z}}{k}{}<0) RequireConcave(i)
            IF (\mp@subsup{\overline{z}}{i}{}>0) RequireConvex(k)
            IF (\mp@subsup{\underline{z}}{i}{}<0) RequireConcave(k)
            ELSE
            IF (颜}>0) RequireConcave(i
            IF (\mp@subsup{\underline{z}}{k}{}<0) RequireConvex(i)
            IF (詨}>0)\mathrm{ RequireConcave(k)
            IF (\mp@subsup{z}{i}{}<0) RequireConvex(k)
            END
            END
        END
    END
END
```

ALGORITHM 5．Subroutine to choose which side of a bilinear interaction to add to $Y$

This subroutine decides which variables in a bilinear interaction of the variables in $L$ on the left hand side and variables in $R$ on the right hand side．For the envelope to be tight in the limit，all the variables from one side must be in $Y$ ．It chooses the side whose variables not already in $Y$ are linked to most other variables．This choice results in the minimum number of variables being added to $Y$ ．

```
set ResolveBilinear(set \(L\), set \(R\) )
\(L^{\prime}:=L \backslash Y\)
\(R^{\prime}:=R \backslash Y\)
IF ( \(\left.L^{\prime}=\emptyset \vee R^{\prime}=\emptyset\right)\) RETURN \(\emptyset\)
\(L^{*}:=\left\{x_{i}: \exists a \in L^{\prime}, \exists(b, c) \in A,\left(x_{i} \in b \wedge a \in c\right) \vee\left(a \in b \wedge x_{i} \in c\right)\right\} \backslash L^{\prime}\)
\(R^{*}:=\left\{x_{i}: \exists a \in R^{\prime}, \exists(b, c) \in A,\left(x_{i} \in b \wedge a \in c\right) \vee\left(a \in b \wedge x_{i} \in c\right)\right\} \backslash R^{\prime}\)
IF ( \(\left|L^{*}\right| \geq\left|R^{*}\right|\) ) RETURN \(L^{\prime}\)
ELSE RETURN \(R^{\prime}\)
```

ALGORITHM 6．Main driver to determine branching variables
When an element of $z$ has a finite upper bound，it requires a tight convex envelope in the relaxation，and likewise when an element of $z$ has a finite lower bound，it requires a tight concave envelope．The main driver makes the necessary additions to $Y$ to provide the necessary tight envelopes for all the constrained elements of $Y$ ．

The driver has two main phases．In the first phase，variables are added to $Y$ based on their role in squared terms and $\xi$ while accumulating information about
the bilinear interactions. In the second phase, the bilinear interactions are resolved. The elements of $A$ must be processed in order of increasing size where the size of an element of $A$ is defined as the maximum of the cardinality of its two component sets. When the argmin used in the algorithm below has more than one element, choose any member.

$$
A:=\emptyset
$$

$$
Y:=\emptyset
$$

FOR $j:=n+1$ TO $N$ BEGIN
$\operatorname{IF}\left(z_{j}^{U}<\infty\right)$ RequireConvex $(j)$
IF $\left(z_{j}^{L}>-\infty\right)$ RequireConcave $(j)$

## END

WHILE $A \neq \emptyset$ BEGIN

```
    \((L, R) \in \operatorname{argmin}_{(a, b) \in A} \max \{|a|,|b|\}\)
    \(Y:=Y \cup\) ChooseBilinear \((L, R)\)
    \(A:=A \backslash\{(L, R)\}\)
```

END

At the end of the main driver, $Y$ contains the set of variables which require branching.

## B. Coefficients for example problems

Table IV. Objective function coefficients for example one

| $i$ | $c_{i}$ | $i$ | $c_{i}$ | $i$ | $c_{i}$ | $i$ | $c_{i}$ |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 1 | -1.066890 | 7 | 0.5149100 | 13 | -0.2178510 | 19 | -1.5776400 |
| 2 | 1.334450 | 8 | 1.6398600 | 14 | 1.0153500 | 20 | 0.0811166 |
| 3 | -1.224840 | 9 | 0.0678508 | 15 | 0.0649806 | 21 | 0.0529182 |
| 4 | -0.534849 | 10 | -0.4161970 | 16 | -1.1314100 | 22 | 1.6965300 |
| 5 | -1.426790 | 11 | 0.5154940 | 17 | 1.8142800 | 23 | -0.4532200 |
| 6 | -0.234014 | 12 | -0.0328012 | 18 | -1.8519400 |  |  |

Table V. Right hand sides for example one

| $i$ | $b_{i}$ | $k$ | $d_{k}$ | $k$ | $d_{k}$ |
| ---: | ---: | ---: | ---: | :---: | ---: |
| 1 | 1.0498000 | 1 | -1.4089100 | 11 | 0.690719 |
| 2 | -0.9275090 | 2 | 1.7586000 | 12 | 1.849930 |
| 3 | -0.0207621 | 3 | 1.6076600 | 13 | -0.281364 |
| 4 | 0.5252870 | 4 | 0.5655480 | 14 | 1.373770 |
| 5 | -0.1074780 | 5 | 1.5045800 | 15 | 0.536129 |
| 6 | 1.0312700 | 6 | -1.4236300 | 16 | 1.664650 |
| 7 | 0.3278110 | 7 | 0.0323101 | 17 | 1.084130 |
| 8 | -1.6362600 | 8 | -1.9086900 | 18 | 0.784348 |
| 9 | 1.0860800 | 9 | 0.7539460 | 19 | 0.618497 |
| 10 | -1.8557600 | 10 | 1.1442900 | 20 | -1.841670 |

Table VI. Nonzero elements of A for example one

| $i$ | $j$ | $A_{i j}$ | $i$ | $j$ | $A_{i j}$ | $i$ | $j$ | $A_{i j}$ |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 1 | 1 | 0.791494 | 4 | 22 | -0.6831560 | 8 | 13 | -0.6074750 |
| 1 | 7 | 1.028900 | 5 | 2 | 1.2722000 | 8 | 18 | 2.3017330 |
| 1 | 12 | 1.253470 | 5 | 9 | 0.8997950 | 8 | 22 | 1.2365400 |
| 1 | 19 | 1.196050 | 5 | 12 | -0.0921251 | 9 | 1 | 1.5216300 |
| 2 | 2 | 0.316459 | 5 | 20 | 1.3299400 | 9 | 9 | 0.0291254 |
| 2 | 7 | -0.767426 | 6 | 9 | 1.2999700 | 9 | 11 | 1.3245300 |
| 2 | 9 | -0.319650 | 6 | 13 | 0.1536300 | 9 | 18 | -1.5178200 |
| 3 | 9 | -1.808227 | 6 | 15 | -1.9864000 | 10 | 7 | -1.6190100 |
| 3 | 21 | 0.573109 | 6 | 20 | -1.8752800 | 10 | 10 | 0.3279450 |
| 3 | 23 | 1.953350 | 7 | 8 | -1.1367900 | 10 | 11 | 1.7859800 |
| 4 | 12 | -0.746296 | 7 | 12 | 0.4287280 | 10 | 22 | 1.4543600 |
| 4 | 15 | -0.650458 | 7 | 16 | -0.7282910 |  |  |  |
| 4 | 19 | 1.764980 | 7 | 18 | -1.8227200 |  |  |  |

Table VII. Nonzero elements of B for example one

| $k$ | $i$ | $j$ | $B_{k i j}$ | $k$ | $i$ | $j$ | $B_{k i j}$ | $k$ | $i$ | $j$ | $B_{k i j}$ |
| ---: | ---: | ---: | :---: | :---: | ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 2 | 3 | 0.5998530 | 6 | 3 | 3 | -1.245270 | 14 | 6 | 2 | 0.8437320 |
| 1 | 4 | 2 | 1.1618200 | 6 | 4 | 2 | 1.070480 | 15 | 17 | 2 | -1.5720900 |
| 1 | 10 | 2 | 0.0968363 | 6 | 8 | 2 | 1.481690 | 15 | 17 | 3 | 1.1675800 |
| 1 | 11 | 1 | 0.5953090 | 7 | 11 | 1 | -0.738157 | 15 | 18 | 1 | -1.2703200 |
| 1 | 12 | 2 | 0.0157741 | 7 | 15 | 2 | -1.998290 | 15 | 20 | 1 | -0.1026120 |
| 1 | 16 | 2 | -0.3495940 | 8 | 3 | 1 | 0.660109 | 16 | 7 | 1 | 1.4422200 |
| 2 | 3 | 2 | 1.5343800 | 8 | 13 | 2 | 0.297381 | 16 | 14 | 2 | 1.4503700 |
| 2 | 8 | 1 | 0.6215500 | 8 | 15 | 1 | 0.753913 | 17 | 3 | 2 | -1.1957700 |
| 2 | 10 | 1 | 1.8293700 | 9 | 1 | 3 | -1.704470 | 17 | 6 | 2 | 1.5247900 |
| 2 | 16 | 2 | -1.1923600 | 9 | 6 | 2 | -0.489378 | 17 | 7 | 2 | 0.7601060 |
| 3 | 5 | 1 | 1.6885800 | 9 | 15 | 2 | -0.588499 | 17 | 18 | 1 | -0.7240830 |
| 3 | 6 | 2 | 1.0501500 | 10 | 11 | 2 | -1.113930 | 18 | 9 | 3 | -1.8605100 |
| 3 | 16 | 3 | 0.0280099 | 11 | 3 | 1 | 1.192800 | 18 | 13 | 3 | -1.0674200 |
| 3 | 17 | 1 | -0.1299910 | 11 | 10 | 3 | 1.908350 | 19 | 16 | 1 | -1.9499800 |
| 4 | 4 | 1 | 0.4644940 | 11 | 13 | 2 | -1.028490 | 19 | 20 | 3 | -1.3409600 |
| 4 | 9 | 3 | -1.0991400 | 11 | 14 | 2 | 1.395810 | 20 | 2 | 1 | -1.8119700 |
| 4 | 11 | 3 | 1.2386100 | 12 | 18 | 3 | -1.569720 | 20 | 7 | 1 | -1.1783800 |
| 4 | 19 | 2 | -0.3364220 | 13 | 5 | 2 | -0.535376 | 20 | 9 | 2 | 0.7480300 |
| 4 | 19 | 3 | 0.9405890 | 13 | 12 | 1 | 0.939518 | 20 | 12 | 2 | 1.4576600 |
| 5 | 10 | 2 | -1.5426700 | 13 | 15 | 2 | -1.577420 | 20 | 17 | 3 | -0.0330721 |
| 5 | 18 | 1 | 1.5738700 | 14 | 1 | 1 | -2.771270 |  |  |  |  |

Table VIII. Variable table for example two

| Var. | Lower bound | Upper bound | Objective coef. |
| ---: | ---: | ---: | ---: |
| $y_{1}$ | 4.828313737302301 | 7.025538314638521 | 0 |
| $y_{2}$ | 4.422848629194137 | 6.620073206530357 | 0 |
| $x_{1}$ | 6.214608098422191 | 8.411832675758411 | 0 |
| $x_{2}$ | 6.214608098422191 | 8.411832675758411 | 0 |
| $x_{3}$ | 6.214608098422191 | 8.411832675758411 | 0 |
| $x_{4}$ | 0 | 165.5545475362379 | $1.191905471317204 \times 10^{-5}$ |
| $x_{5}$ | 0 | 65.55454753623789 | $1.5169705998526 \times 10^{-5}$ |
| $x_{6}$ | 0 | 186.4007582566057 | 0.003342149157327824 |
| $x_{7}$ | 0 | 65.55454753623789 | 0.004253644382053594 |
| $x_{8}$ | 0 | 213.5992417433942 | 0.003342149157327824 |
| $x_{9}$ | 0 | 65.55454753623789 | 0.004253644382053594 |
| $x_{10}$ | 0 | 234.4454524637621 | $1.191905471317204 \times 10^{-5}$ |
| $x_{11}$ | 0 | 65.55454753623789 | $1.51697059985826 \times 10^{-5}$ |
| $x_{12}$ | 0 | 165.5545475362379 | 0.003342149157327824 |
| $x_{13}$ | 0 | 86.40075825660574 | 0.004253644382053594 |
| $x_{14}$ | 0 | 186.4007582566057 | 0.9371515827914514 |
| $x_{15}$ | 0 | 86.40075825660574 | 1.192738378098211 |
| $x_{16}$ | 0 | 213.5992417433942 | 0.9371515827914514 |
| $x_{17}$ | 0 | 86.40075825660574 | 1.192738378098211 |
| $x_{18}$ | 0 | 234.4454524637621 | 0.003342149157327824 |
| $x_{19}$ | 0 | 86.40075825660574 | 0.004253644382053594 |
| $x_{20}$ | 0 | 165.5545475362379 | 0.00334214915732783 |
| $x_{21}$ | 0 | 113.5992417433942 | 0.004253644382053602 |
| $x_{22}$ | 0 | 186.4007582566057 | 0.9371515827914529 |
| $x_{23}$ | 0 | 113.5992417433942 | 1.192738378098213 |
| $x_{24}$ | 0 | 213.5992417433942 | 0.9371515827914529 |
| $x_{25}$ | 0 | 113.5992417433942 | 1.192738378098213 |
| $x_{26}$ | 0 | 234.4454524637621 | 0.00334214915732783 |
| $x_{27}$ | 0 | 113.5992417433942 | 0.004253644382053602 |
| $x_{28}$ | 0 | 165.5545475362379 | $1.191905471317204 \times 10^{-5}$ |
| $x_{29}$ | 0 | 134.4454524637621 | $1.5169705998526 \times 10^{-5}$ |
| $x_{30}$ | 0 | 186.4007582566057 | 0.003342149157327824 |
| $x_{31}$ | 0 | 134.4454524637621 | 0.004253644382053594 |
| $x_{32}$ | 0 | 213.5992417433942 | 0.003342149157327824 |
| $x_{33}$ | 0 | 134.4454524637621 | 0.004253644382053594 |
| $x_{34}$ | 0 | 234.4454524637621 | $1.191905471317204 \times 10^{-5}$ |
| $x_{35}$ | 0 | 134.4454524637621 | $1.51697059985826 \times 10^{-5}$ |
|  |  |  |  |

Table IX. Objective coefficients for example three

| Var. | Coef. | Var. | Coef. | Var. | Coef. |
| ---: | ---: | ---: | ---: | ---: | ---: |
| $y_{1}$ | -0.4000 | $x_{6}$ | -0.9196 | $x_{14}$ | -0.0108 |
| $y_{2}$ | -0.5000 | $x_{7}$ | -0.2165 | $x_{15}$ | -0.8976 |
| $y_{3}$ | -0.6000 | $x_{8}$ | -0.0944 | $x_{16}$ | -0.8341 |
| $x_{1}$ | -0.4239 | $x_{9}$ | -0.8582 | $x_{17}$ | -0.7077 |
| $x_{2}$ | -0.9664 | $x_{10}$ | -0.0174 | $x_{18}$ | -0.6108 |
| $x_{3}$ | -0.4955 | $x_{11}$ | -0.6566 | $x_{19}$ | -0.7102 |
| $x_{4}$ | -0.8139 | $x_{12}$ | -0.2996 | $x_{20}$ | -0.2678 |
| $x_{5}$ | -0.8432 | $x_{13}$ | -0.2621 |  |  |

## C. Solution for example problems

Table X. Solution of example one

| Var. | Value | Var. | Value | Var. | Value |
| :--- | ---: | ---: | ---: | :---: | ---: |
| $y_{1}$ | -0.6032 | $x_{6}$ | 0.1085 | $x_{14}$ | -1.2352 |
| $y_{2}$ | -1.9003 | $x_{7}$ | 2.0000 | $x_{15}$ | -0.0395 |
| $y_{3}$ | 2.0000 | $x_{8}$ | -2.0000 | $x_{16}$ | 0.0899 |
| $x_{1}$ | 0.9258 | $x_{9}$ | -0.4036 | $x_{17}$ | -2.0000 |
| $x_{2}$ | 1.4371 | $x_{10}$ | -1.5271 | $x_{18}$ | -0.5893 |
| $x_{3}$ | 2.0000 | $x_{11}$ | -2.0000 | $x_{19}$ | -2.0000 |
| $x_{4}$ | 1.8715 | $x_{12}$ | 2.0000 | $x_{20}$ | -0.2627 |
| $x_{5}$ | -1.6586 | $x_{13}$ | 2.0000 | Objective | -20.8008 |

Table XI. Solution of example two

| Var. | Value | Var. | Value | Var. | Value |
| :---: | ---: | :---: | ---: | :---: | ---: |
| $y_{1}$ | 6.7795 | $x_{12}$ | 165.56 | $x_{25}$ | 86.40 |
| $y_{2}$ | 6.0863 | $x_{13}$ | 86.40 | $x_{26}$ | 234.46 |
| $x_{1}$ | 7.4726 | $x_{14}$ | 186.40 | $x_{27}$ | 73.37 |
| $x_{2}$ | 7.8781 | $x_{15}$ | 86.40 | $x_{28}$ | 165.56 |
| $x_{3}$ | 8.1658 | $x_{16}$ | 213.60 | $x_{29}$ | 116.43 |
| $x_{4}$ | 165.56 | $x_{17}$ | 86.40 | $x_{30}$ | 186.40 |
| $x_{5}$ | 65.55 | $x_{18}$ | 234.46 | $x_{31}$ | 103.40 |
| $x_{6}$ | 186.40 | $x_{19}$ | 73.37 | $x_{32}$ | 213.60 |
| $x_{7}$ | 65.55 | $x_{20}$ | 165.56 | $x_{33}$ | 86.40 |
| $x_{8}$ | 213.60 | $x_{21}$ | 113.60 | $x_{34}$ | 234.46 |
| $x_{9}$ | 65.55 | $x_{22}$ | 186.40 | $x_{35}$ | 73.37 |
| $x_{10}$ | 234.46 | $x_{23}$ | 103.40 | Objective | -183.29 |
| $x_{11}$ | 65.55 | $x_{24}$ | 213.60 |  |  |

Table XII. Solution of example three

| Var. | Value | Var. | Value | Var. | Value |
| :---: | ---: | :---: | :---: | :---: | ---: |
| $y_{1}$ | -2.0000 | $x_{6}$ | 2.6414 | $x_{14}$ | 0.0261 |
| $y_{2}$ | 0.6019 | $x_{7}$ | 0.6219 | $x_{15}$ | 2.1703 |
| $y_{3}$ | 1.8981 | $x_{8}$ | 0.2712 | $x_{16}$ | 2.0167 |
| $x_{1}$ | 1.2176 | $x_{9}$ | 2.0750 | $x_{17}$ | 1.7065 |
| $x_{2}$ | 2.7759 | $x_{10}$ | 0.0421 | $x_{18}$ | 1.4728 |
| $x_{3}$ | 1.4233 | $x_{11}$ | 1.5876 | $x_{19}$ | 1.7125 |
| $x_{4}$ | 2.3378 | $x_{12}$ | 0.7244 | $x_{20}$ | 0.6458 |
| $x_{5}$ | 2.4220 | $x_{13}$ | 0.6337 | Objective | -21.412 |

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