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Modeling of discrete/continuous optimization problems: characterization and formulation of disjunctions and their relaxations

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Abstract

This paper addresses the relaxations in alternative models for disjunctions, big-M and convex hull model, in order to develop guidelines and insights when formulating Mixed-Integer Non-Linear Programming (MINLP), Generalized Disjunctive Programming (GDP), or hybrid models. Characterization and properties are presented for various types of disjunctions. An interesting result is presented for improper disjunctions where results in the continuous space differ from the ones in the mixed-integer space. A cutting plane method is also proposed that avoids the explicit generation of equations and variables of the convex hull. Several examples are presented throughout the paper, as well as a small process synthesis problem, which is solved with the proposed cutting plane method.

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1. Introduction

Developing optimization models with discrete and continuous variables is not a trivial task. The modeler has often several alternative formulations for the same problem, and each of them can have a very different performance in the efficiency on the problem solution. In the area of Process System Engineering models commonly involve linear and nonlinear constraints and discrete choices. The traditional model that has been used in the past corresponds to a mixed-integer optimization program whose representation can be expressed in the following equation form (Grossmann & Kravanja, 1997):

$$\begin{aligned} \min Z &= f(x) + d^T y \\ \text{s.t. } g(x) &\leq 0 \quad (\text{PA}) \\ r(x) + Ly &\leq 0 \\ Ay &\geq a \end{aligned}$$

$$x \in R^n, \quad y \in \{0, 1\}^q$$

where $f(x)$, $g(x)$ and $r(x)$ are linear and/or nonlinear functions. In the model (PA) the discrete choices are represented with the binary variables y involving linear terms.

More recently, generalized disjunctive programming (Raman & Grossmann, 1994; Türkay & Grossmann, 1996) has been proposed as an alternative to the model (PA). A generalized disjunctive program can be formulated as follows:

$$\min Z = \sum_{k \in K} c_k + f(x)$$

$$\text{s.t. } g(x) \leq 0$$

$$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(x) \leq 0 \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K \quad (\text{GDP})$$

$$\Omega(Y) = \text{True}$$

$$x \in R^n, \quad Y_{ik} \in \{\text{True}, \text{False}\}^m, \quad c_k \geq 0$$

where the discrete choices are expressed with the Boolean variables Y_{ik} in terms of disjunctions, and logic propositions $\Omega(Y)$. The attractive feature of Generalized Disjunctive Programming (GDP) is that it allows a

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symbolic/quantitative representation of discrete and continuous optimization problems. Modeling language for GDP problem has been discussed by Vecchiotti and Grossmann (2000).

An approach that combines the previous two models is a hybrid model proposed by Vecchiotti and Grossmann (1999) where the discrete choices can be modeled as mixed-integer constraints and/or disjunctions. In this way we can potentially exploit the advantages of the two previous formulations by expressing part of it only in algebraic form, and the other in a symbolic/quantitative form. The hybrid formulation is as follows:

$$\min Z = \sum_{k \in K} c_k + f(x) + d^T y$$

$$\text{s.t. } g(x) \leq 0$$

$$r(x) + Ly \leq 0$$

$$Ay \geq a \quad (\text{PH})$$

$$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(x) \leq 0 \\ c_k = y_{ik} \end{bmatrix} \quad k \in K$$

$$\Omega(Y) = \text{True}$$

$$x \in R^n, \quad y \in \{0, 1\}^q, \quad Y_{ik} \in \{\text{True}, \text{False}\}^m, \quad c_k \geq 0$$

where $r(x) + Ly \leq 0$ is general mixed-integer constraints that can be linear/nonlinear equations/inequalities. These terms can be seen as disjunctions transformed into mixed-integer form. $Ay \geq a$ represents general integer equalities/inequalities transformed from former logic propositions.

An issue that is unclear is how the modeler should express the discrete choices, either as a symbolic disjunction, or in a mixed-integer form (Bockmayr & Kasper, 1998). One possible guideline for this decision is the gap between the optimal value of the continuous relaxation and the optimal integer value. Since several algorithms involve the solution of the relaxed problem, we will investigate in this paper the tightness of different relaxations for a disjunctive set: the big-M formulation (Nemhauser & Wolsey, 1988), the Beaumont surrogate (Beaumont, 1990) and the convex hull relaxation (Balas, 1979; Lee & Grossmann, 2000). The big-M formulation and the Beaumont surrogate can be regarded as ‘obvious’ constraints. However, the convex hull relaxation of a disjunction is tighter, and can be transformed into a set of mixed-integer constraints. The advantage of the convex hull relaxation is that the tight lower bound helps to reduce the search effort in the branch and bound procedure, in both nonlinear and linear problems (for examples of significant node reductions see Lee & Grossmann, 2000; Jackson & Grossmann, 2002). But the drawback with the convex hull formulation is that it increases the number of continuous variables and constraints of the original problem. This can potentially make a problem more expensive to solve, especially in

large problems. The big-M relaxation is more convenient to use when the problem size does not increase substantially when compared with the convex hull relaxation (see Yeomans & Grossmann, 1999, who found the big-M to be more effective). But generally the lower bound by big-M relaxation is weaker, which may require longer CPU time than the convex hull relaxation. Therefore, depending on the case, there is a trade-off between the best possible relaxation and the problem size. In order to exploit the tightness of the convex hull relaxation, but without the substantial increase of the constraints, it will be shown that cutting planes can be used that correspond to a facet of the convex hull.

In this paper we first introduce the definition and properties of a disjunctive set. We then present the different relaxations and their properties. Finally, a cutting plane method is discussed, and illustrated with several small example problems. The goal of this paper is not to perform a detailed computational study, but rather to provide insights into the modeling and solution of disjunctive problems.

2. Definitions and properties of a disjunctive set

A disjunctive set F can be expressed as a set of constraints separated by the or (\vee) operator:

$$F = \bigvee_{i \in D} [h_i(x) \leq 0] \quad x \in R^n \quad (1)$$

It is assumed that $h_i(x)$ is a continuous convex function. F can be considered as a logical expression, which enforces only one set of inequalities. The feasible region of each disjunctive term can be expressed as the set of points that satisfy the inequality.

$$R_i = \{x | h_i(x) \leq 0\} \quad (2)$$

A disjunctive set can be expressed in other forms that are logically equivalent. F can also be expressed as the union of the feasible regions of the disjunctive terms, which is called Disjunctive Normal Form (DNF):

$$F = \bigcup_{i \in D} [h_i(x) \leq 0] \quad x \in R^n \quad (3)$$

$$F = \bigcup_{i \in D} R_i \quad (4)$$

If the union of the feasible regions of the disjunctive terms is equal to one of its terms, R_j , which is the largest feasible region, then the disjunctive set is called *improper*. Otherwise the disjunctive set is called *proper* (Balas, 1985). The *improper* disjunctive set can be written as follows:

$$F = \bigcup_{i \in D} R_i = R_j \quad (5)$$

The *improper* disjunctive set has also the following property:

$$153 \quad R_i \subseteq R_j \quad \forall i \neq j \quad (6)$$

154 which means that the feasible regions i ($i \neq j$) in the
155 disjunctive set F are included in the j th feasible region.
156 Since F is expressed as the union of the different terms,
an *improper* disjunctive set can be reduced to:

$$157 \quad F = \{x | h_j(x) \leq 0\} \quad (7)$$

On the other hand, a *proper* disjunctive set is the one
158 in which either the intersection of the feasible regions is
159 empty, or else it is non-empty, but Eq. (5) does not
160 apply. Therefore, for a *proper* disjunctive set, either
161 there is no intersection among the feasible regions:

$$162 \quad \bigcap_{i \in D} R_i = \emptyset \quad (8)$$

or else, there is some intersection, but no set R_j contains
163 all of them:

$$164 \quad \bigcap_{i \in D} R_i \neq \emptyset, \quad \bigcup_{i \in D} R_i \neq R_j \quad (9)$$

165 3. Relaxations of a disjunctive set

166 Given a disjunctive set as condition Eq. (1) there are a
167 number of relaxations that can be derived, the big-M,
168 the Beaumont surrogate and the convex hull relaxations.
169 We consider below the case of convex nonlinear con-
170 straints, which easily simplifies to the linear case.

171 3.1. Big-M relaxation

172 Consider the following nonlinear disjunction:

$$173 \quad F = \bigvee_{i \in D} [h_i(x) \leq 0] \quad x \in R^n \quad (10)$$

174 where $h_i(x)$ is a nonlinear convex function. For simpli-
175 city, and without loss of generality, it is assumed that
176 each term in the disjunction Eq. (10) has only one
177 inequality constraint. The big-M relaxation of Eq. (10)
is given by:

$$178 \quad h_i(x) \leq M_i(1 - y_i) \quad i \in D$$

$$\sum_{i \in D} y_i = 1$$

$$179 \quad 0 \leq y_i \leq 1, \quad i \in D \quad (11)$$

Again the tightest value for M_i can be calculated
179 from:

$$180 \quad M_i = \max\{h_i(x) | x^L \leq x \leq x^U\} \quad (12)$$

3.2. Beaumont relaxation

181
182 **Beaumont (1990)** proposed a valid inequality for the
183 disjunctive set Eq. (10). A valid M_i value must be
184 calculated as in Eq. (12). By dividing each constraint $i \in$
185 D in Eq. (11) by M_i and summing over $i \in D$, the
186 Beaumont surrogate, which interestingly does not in-
187 involve binary variables is given as follows:

$$\sum_{i \in D} \frac{h_i(x)}{M_i} \leq N - 1 \quad (13) \quad 188$$

where $N = |D|$ in Eq. (10). Beaumont showed that Eq.
189 (13) yields an equivalent relaxation as the big-M
190 relaxation Eq. (11) projected onto the continuous x
191 space when the constraints in Eq. (10) are linear.

3.3. Convex hull relaxation

192
193 The convex hull relaxation for the disjunctive set Eq.
194 (10) can be written as follows (Lee & Grossmann, 2000):

$$x - \sum_{i \in D} v_i = 0 \quad x, v_i \in R^n \quad 195$$

$$y_i h_i \left(\frac{v_i}{y_i} \right) \leq 0, \quad i \in D$$

$$\sum_{i \in D} y_i = 1$$

$$0 \leq y_i \leq 1 \quad i \in D$$

$$0 \leq v_i \leq v_i^U y_i, \quad i \in D \quad (14)$$

196 where v_i^U is a valid upper bound for the disaggregated
197 variables v_i , usually chosen as x^U . The Eq. (14) define a
198 convex set in the (x, v, y) space provided the inequalities
199 $h_i(x) \leq 0, i \in D$ are convex and bounded. The convex
200 hull in Eq. (14) can be proved to be tighter or at least as
201 tight as the big-M relaxation (see Appendix A). Also, for
202 case of linear disjunctions, $F = \bigvee_{i \in D} [a_i^T x \leq b_i] \quad x \in R^n$,
Eq. (14) reduces to the equations by Balas (1979, 1988):

$$x - \sum_{i \in D} v_i = 0 \quad x, v_i \in R^n \quad 203$$

$$a_i^T v_i - b_i y_i \leq 0, \quad i \in D$$

$$\sum_{i \in D} y_i = 1$$

$$0 \leq y_i \leq 1, \quad i \in D$$

$$0 \leq v_i \leq y_i v_i^{\text{up}}, \quad i \in D \quad (15)$$

204 3.4. Example 1

205 Consider the following nonlinear disjunction:

206
$$[(x_1 - 1)^2 + (x_2 - 1)^2 \leq 1] \vee [(x_1 - 4)^2 + (x_2 - 2)^2 \leq 1]$$

$$\vee [(x_1 - 2)^2 + (x_2 - 4)^2 \leq 1]$$

207 where $0 \leq x_1 \leq 5$ and $0 \leq x_2 \leq 5$. The feasible region is
208 shown in Fig. 1. Figs. 2 and 3 show the feasible region of
209 the big-M and the convex hull relaxations, respectively.

210 The big-M relaxation is given by:

211
$$(x_1 - 1)^2 + (x_2 - 1)^2 \leq 1 + 31(1 - y_1)$$

$$(x_1 - 4)^2 + (x_2 - 2)^2 \leq 1 + 24(1 - y_2)$$

$$(x_1 - 2)^2 + (x_2 - 4)^2 \leq 1 + 24(1 - y_3)$$

$$y_1 + y_2 + y_3 = 1$$

$$0 \leq x_1, x_2 \leq 5, \quad 0 \leq y_i \leq 1, \quad i = 1, 2, 3 \quad (16)$$

212 where the big-M parameters are calculated by Eq. (12).

213 The convex hull of Fig. 3 is given by the equations:

$$x_1 = v_{11} + v_{12} + v_{13}$$

$$x_2 = v_{21} + v_{22} + v_{23}$$

$$(y_1 + \varepsilon) \left[\left(\frac{v_{11}}{y_1 + \varepsilon} - 1 \right)^2 + \left(\frac{v_{21}}{y_1 + \varepsilon} - 1 \right)^2 - 1 \right] \leq 0$$

$$(y_2 + \varepsilon) \left[\left(\frac{v_{12}}{y_2 + \varepsilon} - 4 \right)^2 + \left(\frac{v_{22}}{y_2 + \varepsilon} - 2 \right)^2 - 1 \right] \leq 0$$

$$(y_3 + \varepsilon) \left[\left(\frac{v_{13}}{y_3 + \varepsilon} - 2 \right)^2 + \left(\frac{v_{23}}{y_3 + \varepsilon} - 4 \right)^2 - 1 \right] \leq 0$$

$$y_1 + y_2 + y_3 = 1$$

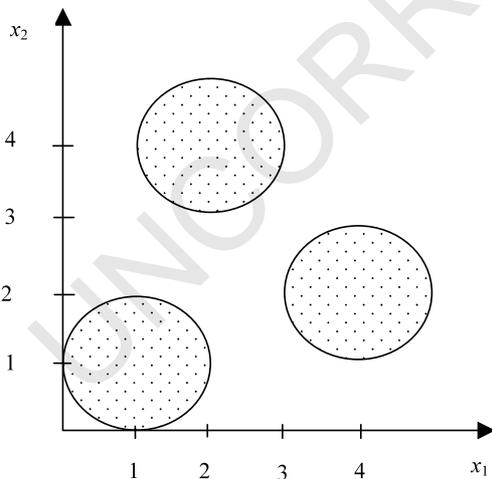


Fig. 1. Feasible region of example 1.

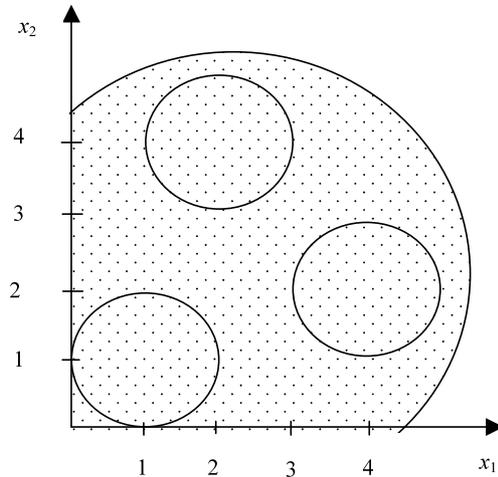


Fig. 2. Big-M relaxation of example 1.

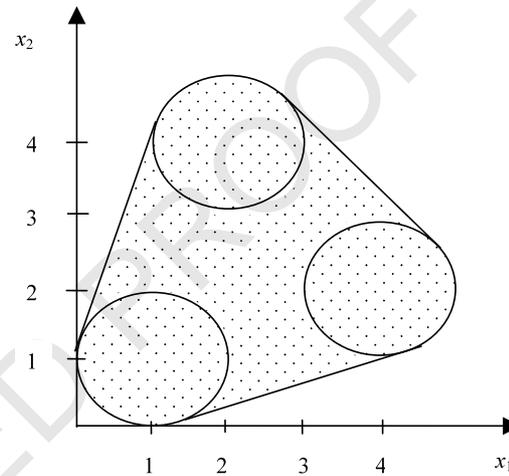


Fig. 3. Convex hull relaxation of example 1.

$$0 \leq y_i \leq 1, \quad i = 1, 2, 3$$

$$0 \leq v_{ji} \leq 5y_i \quad \forall i, \forall j \quad (17)$$

Note that to avoid division by zero ε is introduced in the nonlinear inequalities as a small tolerance (Lee & Grossmann, 2000). Typical values for ε are 0.001–0.0001. From Figs. 2 and 3 it is clear that the convex hull relaxation of the disjunctive set is tighter than the big-M relaxation for this example.

4. Impact of nature of disjunctions on relaxations in x space

Our aim in this section is to analyze different types of disjunctions for which it may be convenient or not to transform them into the convex hull formulation or a big-M formulation or Beaumont surrogate. Since the big-M formulation is as tight as the Beaumont surrogate, and it is more frequently used, we will compare the

convex hull with only the big-M formulation. We will analyze the following cases: (a) *improper* disjunction; (b) *proper* disjunction. Within this last case we will analyze when the intersection of the feasible regions is empty and when it is non-empty.

If we denote the feasible region of the convex hull relaxation in the continuous x space as R_{CH} , the feasible region of the big-M relaxation as R_{BM} , and the feasible region of the Beaumont surrogate as R_B , then according to the properties shown in the previous section, the following can be established:

$$R_{CH} \subseteq R_{BM} \quad (18)$$

Beaumont (1990) has shown for the linear case that $R_{BM} = R_B$ where R_B is defined by constraint Eq. (13). In the Appendix A we show that $R_{BM} \subseteq R_B$ for nonlinear case. Therefore, the following property holds:

$$R_{BM} \subseteq R_B \quad (19)$$

It should be noted that properties Eqs. (19) and (20) apply in the space of the continuous variables x .

4.1. Improper disjunction

When the disjunctive set is *improper*, the property in Eq. (6) holds. Since the feasible region of one term contains the feasible regions of the other terms, the relaxations of the convex hull and of the big-M can be selected to be identical. The reason is that the redundant terms can be dropped and the disjunctive set can be represented by the term with the largest feasible region R_j . For example, suppose we have the following problem:

$$\min Z = (x_1 - 3.5)^2 + (x_2 - 4.5)^2$$

$$\text{s.t.} \quad \begin{bmatrix} Y_1 \\ 1 \leq x_1 \leq 3 \\ 2 \leq x_2 \leq 4 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ 2 \leq x_1 \leq 3 \\ 3 \leq x_2 \leq 4 \end{bmatrix} \quad (20)$$

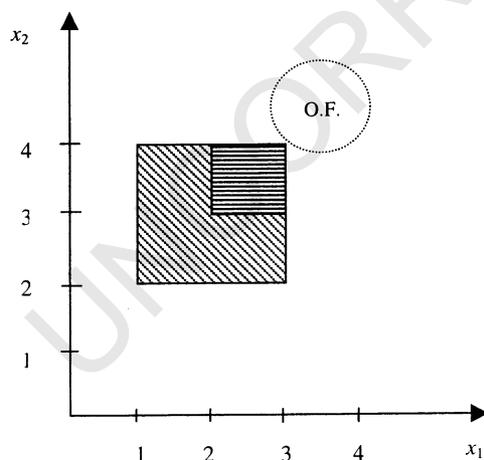


Fig. 4. Feasible region of disjunctive set Eq. (20).

The feasible region is shown in Fig. 4. Choosing the term with the largest feasible region, which is the first one, and solving the problem as an NLP we obtain the optimal solution $x = (3, 4)$ and $Z = 0.5$. If we are not aware that the feasible regions are overlapped we can generate the big-M relaxation for this problem. If we use $M_i = 0.5$, $i = 1, 2$, and solve the relaxed Mixed-Integer Non-Linear Programming (MINLP) problem, the solution is $x = (3.25, 4.25)$, $Z = 0.125$, $y = (0.5, 0.5)$. If we choose $M_i = 1$ and solve the relaxed MINLP then the solution is $x = (3.5, 4.5)$, $Z = 0$, $y = (0.5, 0.5)$. Therefore, it is clear that arbitrary choice of M_i can yield a relaxation whose feasible region is larger than the disjunctive term with the largest feasible region. For the convex hull formulation it is clear that the resulting relaxation coincides with the region of the largest term in the x space, but at the expense of expressing it through disaggregated variables and additional constraints.

4.2. Proper disjunction

4.2.1. Non-empty intersecting feasible regions

When the feasible regions of the disjunctive terms have an intersection, it is not clear whether or not the convex hull and the big-M formulation could yield the same relaxation. Suppose we have disjunctions whose feasible regions are shown in Figs. 5 and 6. In Fig. 5 it is clear that the big-M relaxation, with a good selection of the M_i values can yield the same relaxation as the convex hull. For the case of Fig. 6 the convex hull will yield a tighter relaxation.

4.2.2. Disjoint disjunction

If the feasible region defined by each term in the disjunction has no intersection with others, then the disjunction is disjoint and *proper*. Fig. 7 shows an example of disjoint disjunction. In this case, it is clear that the convex hull relaxation should generally be

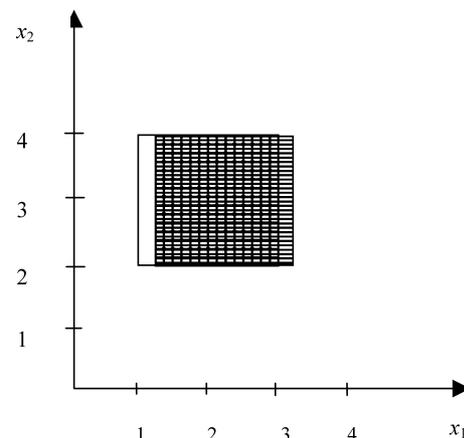


Fig. 5. Intersecting disjunction.

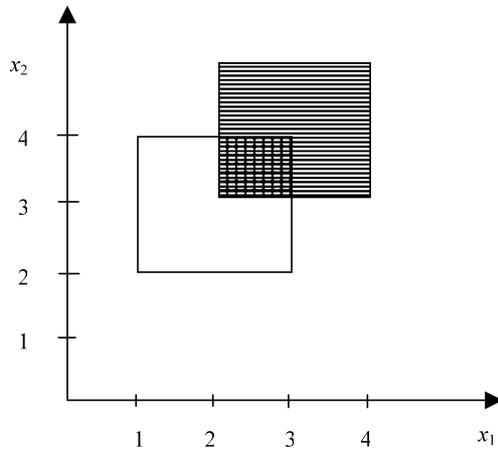


Fig. 6. Intersecting disjunction.

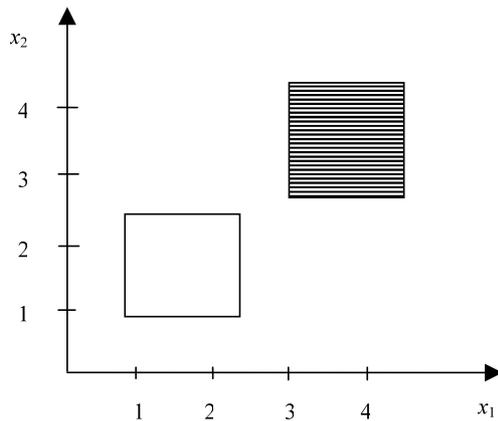


Fig. 7. Disjoint disjunction (general case).

290 tighter than the big-M relaxation (an exception is the
 291 particular case shown in Fig. 8). Also, in the special case
 292 shown in Fig. 9, where a disjunction has two terms with
 293 linear constraints and one of them yields zero point as a
 294 feasible region, the convex hull yields a cone with the
 295 zero point as the vertex. In this case, the convex hull
 296 relaxation can be simplified by not requiring disaggre-
 297 gated variables as given by the following:

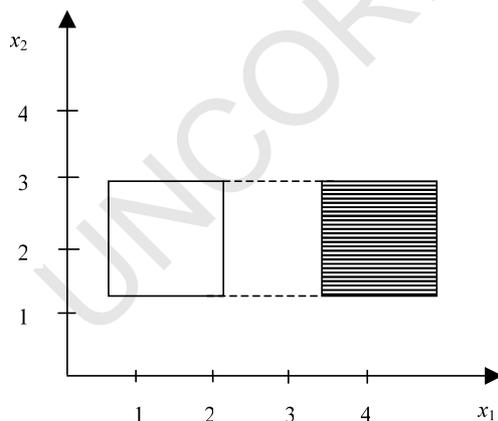


Fig. 8. Disjoint disjunction (particular case).

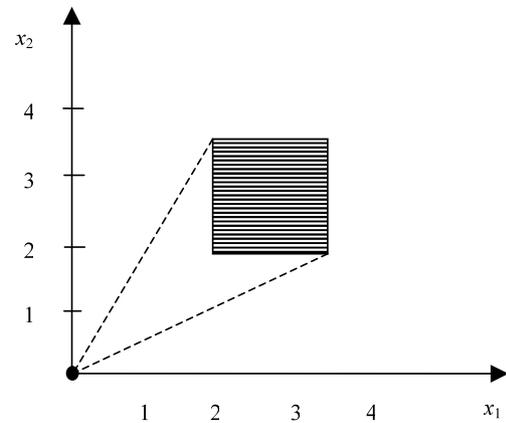


Fig. 9. Disjoint disjunction with zero point.

$$y_1 h_1 \left(\frac{x}{y_1} \right) \leq 0 \quad 298$$

$$0 \leq x \leq x^U y_1$$

$$0 \leq y_1 \leq 1 \quad (21)$$

which includes the zero point as a feasible point. The
 above also applies to linear case. 299

5. Relaxation in x - y space 300

The previous section analyzed the relation of relaxa-
 tions for different types of disjunctions in the x space.
 When applying the big-M constraints Eq. (11) or the
 convex hull Eq. (14) these are written in the x - y space.
 Therefore, an interesting question is whether or not the
 properties we noted in the previous section still apply in
 the x - y space. Let us consider the following example,
 which has an *improper* disjunction. 308

5.1. Example 2 309

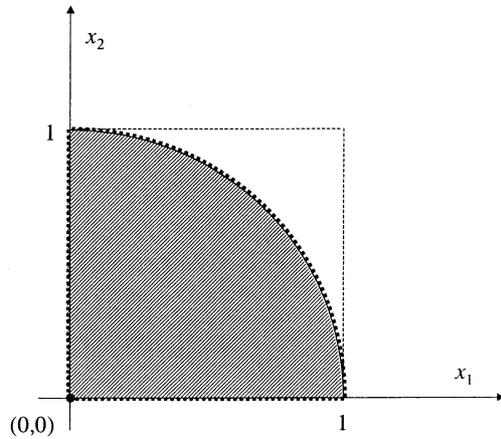
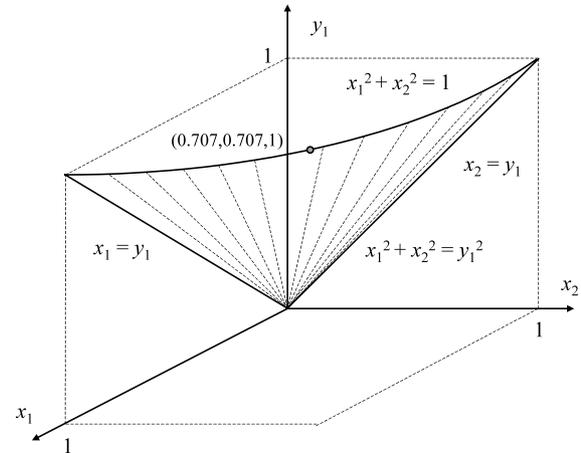
$$\min Z = (x_1 - 1.1)^2 + (x_2 - 1.1)^2 + c_1 \quad 310$$

$$\text{s.t.} \quad \begin{bmatrix} Y_1 \\ x_1^2 + x_2^2 \leq 1 \\ c_1 = 1 \end{bmatrix} \vee \begin{bmatrix} \neg Y_1 \\ x_1 = x_2 = 0 \\ c_1 = 0 \end{bmatrix} \quad 311$$

$$0 \leq x_1, x_2 \leq 1; \quad 0 \leq c_1$$

$$Y_1 \in \{\text{true}, \text{false}\} \quad (22)$$

The optimal solution is $x = (0.707, 0.707)$, $Y_1 = \text{true}$
 and $Z = 1.309$. The feasible region is shown in Fig. 10
 and the feasible region of the second term, which is $(0, 0)$,
 is included in the feasible region of the first term.
 According to the previous section since this is an
improper disjunction in the x space, it ought to be
 sufficient to use the first term only. However, when 317

Fig. 10. Feasible region of example 2 in the x space.Fig. 11. Convex hull relaxation of example 2 in the x - y space.

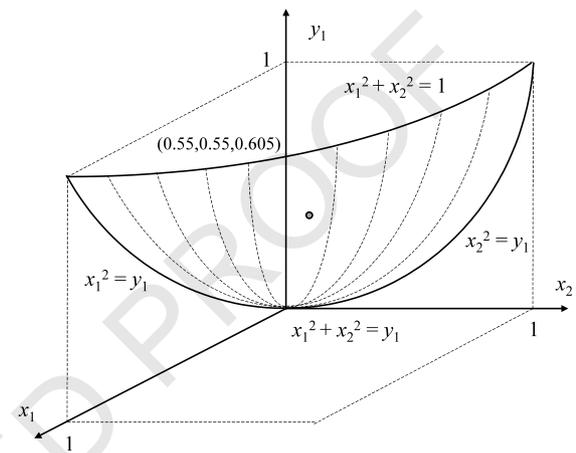
318 expressed algebraically, the big-M relaxation and the
 319 convex hull relaxation of the disjunction in Eq. (23)
 320 involve the additional variable y_1 as a continuous
 321 variable. In the case of the convex hull, we apply Eq.
 322 (22) to the first term. Rearranging the inequality $y_1[(x_1/
 323 y_1)^2 + (x_2/y_1)^2 - 1] \leq 0$ yields:

$$\begin{aligned}
 324 \quad \min Z &= (x_1 - 1.1)^2 + (x_2 - 1.1)^2 + y_1 \\
 &\text{s.t. } x_1^2 + x_2^2 \leq y_1^2 \\
 &0 \leq x_1 \leq y_1 \\
 &0 \leq x_2 \leq y_1 \\
 &0 \leq y_1 \leq 1
 \end{aligned} \tag{23}$$

325 The big-M relaxation of Eq. (23) for the first term is
 given by:

$$\begin{aligned}
 326 \quad \min Z &= (x_1 - 1.1)^2 + (x_2 - 1.1)^2 + y_1 \\
 &\text{s.t. } x_1^2 + x_2^2 \leq y_1 \\
 &0 \leq x_1, x_2 \leq 1; \quad 0 \leq y_1 \leq 1
 \end{aligned} \tag{24}$$

327 Figs. 11 and 12 show the convex hull relaxation and
 328 the big-M relaxation of Eq. (23) in the x - y space,
 329 respectively. It is clear that Eqs. (24) and (25) are not
 330 identical due to the difference in the right hand side of
 331 the nonlinear inequality. In fact, the solution of Eq. (24)
 332 is $(x, y) = (0.707, 0.707, 1)$ and $Z = 1.309$. Since the
 333 relaxed value of y_1 is 1, this solution is the optimal
 334 solution of Eq. (33), which is also shown in Fig. 11. On
 335 the other hand, the solution of Eq. (25) is $(x, y) = (0.55,
 336 0.55, 0.605)$ and $Z = 1.21$ which is weaker than the
 337 convex hull relaxation. This result can be seen by
 338 comparing Figs. 11 and 12. There is no difference
 339 between the feasible set of Eq. (24) and the feasible set
 340 of Eq. (25) projected in the x space as shown in Fig. 10.
 341 The difference, however, takes place in the x - y space.
 Note that the nonlinear constraint in Eq. (25), $x_1^2 + x_2^2 \leq$

Fig. 12. Big-M relaxation of example 2 in the x - y space.

342 y_1 , which is shown in Fig. 12, is weaker than $x_1^2 + x_2^2 \leq y_1^2$
 343 in Eq. (24) for $0 \leq y_1 \leq 1$. Therefore, even though the
 344 disjunction in Eq. (23) is *improper* in x space, the convex
 345 hull yields tighter relaxation than big-M relaxation in
 346 the x - y space. Thus, this example demonstrates that for
 347 the case of *improper* nonlinear disjunctions, the convex
 348 hull may be tighter than the big-M constraint in the x - y
 349 space even if they are identical in the projected x space.

350 For the linear case, we change the nonlinear con-
 351 straint in the first term of the disjunction Eq. (23) by the
 352 following linear constraint:

$$\min Z = (x_1 - 1.1)^2 + (x_2 - 1.1)^2 + c_1 \tag{25}$$

$$\text{s.t. } \begin{bmatrix} Y_1 \\ x_1 + x_2 \leq 1 \\ c_1 = 1 \end{bmatrix} \vee \begin{bmatrix} \neg Y_1 \\ x_1 = x_2 = 0 \\ c_1 = 0 \end{bmatrix}$$

$$0 \leq x_1, x_2 \leq 1; \quad 0 \leq c_1$$

$$Y_1 \in \{\text{true}, \text{false}\} \tag{25}$$

354 where the disjunction is *improper* in the x space. The
 optimal solution is $x = (0.5, 0.5)$, $Y_1 = \text{true}$ and $Z = 1.72$.

355 The convex hull of the disjunction Eq. (26) yields a
356 linear constraint:

$$357 \quad x_1 + x_2 \leq y_1 \quad (26)$$

358 After replacing the disjunction Eq. (26) with convex
359 hull relaxation Eq. (27), the solution is $x = (0.5, 0.5)$,
360 $y_1 = 1$ and $Z = 1.72$, which is exactly the optimal
361 solution of Eq. (26). Since the disjunction Eq. (26) is
362 *improper* in x space, only the first term is sufficient for
363 the relaxation. The big-M relaxation of Eq. (26) is given
364 by:

$$364 \quad x_1 + x_2 - 1 \leq M_1(1 - y_1) \quad (27)$$

365 This relaxation clearly depends on M_1 value. For
366 example, if $M_1 = 1$ is used, then the relaxation yields
367 $x = (0.67, 0.67)$, $y_1 = 0.67$ and $Z = 1.042$, which is weaker
368 than the convex hull relaxation. The best M_1 value in
369 this case is -1 , which yields exactly the same solution as
370 the convex hull relaxation. As shown with this example,
371 even for the linear *improper* disjunction the big-M
372 relaxation may have weaker relaxation than the convex
373 hull depending on the big-M parameter value.

373 6. Cutting plane method

374 The two previous sections have analyzed the issue of
375 determining in what cases it is worth to formulate
376 disjunctions with the convex hull relaxation in order to
377 obtain tighter relaxations when compared with the big-
378 M relaxation. In this section, we present a numerical
379 procedure for generating cutting planes, which poten-
380 tially has the advantage of requiring much fewer
381 variables and constraints than the convex hull relaxa-
382 tion. Cutting planes, which correspond to facets of the
383 convex hull, can improve the tightness of the big-M
384 relaxation. The proposed cutting planes can be used
385 within a branch and cut enumeration procedure (Stubbs
386 & Mehrotra, 1999), or as a way to strengthen an
387 algebraic MINLP model before solving it with one of
388 the standard methods.

389 Using as a basis the GDP model, the general form of
390 the strengthened MINLP model (PC_n) at any iteration n
391 will be as follows:

$$392 \quad \min Z = \sum_{k \in K} \sum_{i \in D_k} \gamma_{ik} y_{ik} + f(x)$$

$$393 \quad \text{s.t. } g(x) \leq 0$$

$$394 \quad h_{ik}(x) \leq M_{ik}(1 - y_{ik}), \quad i \in D_k, \quad k \in K \quad (PC_n)$$

$$395 \quad \sum_{i \in D_k} y_{ik} = 1, \quad k \in K$$

$$396 \quad Ay \leq a$$

$$397 \quad \beta_n^T x \leq b_n, \quad n = 1, 2, \dots, N$$

$$398 \quad x \in R^n, \quad y_{ik} \in \{0, 1\}$$

where $\beta_n^T x \leq b_n$ is the cutting plane at the iteration n .
Let us denote the solution of the continuous relaxation
of (PC_n) as $x_R^{BM,n}$. In order to generate the cutting plane
we consider the following separation problem, which
has as an objective to find the point within the convex
hull that is closest to the point $x_R^{BM,n}$. This separation
problem is given by the NLP:

$$406 \quad \min \phi(x) = (x - x_R^{BM,n})^T (x - x_R^{BM,n}) \quad 406$$

$$407 \quad \text{s.t. } g(x) \leq 0 \quad 407$$

$$408 \quad x = \sum_{i \in D_k} v_{ik}, \quad k \in K \quad 408$$

$$409 \quad y_{ik} h_{ik} \left(\frac{v_{ik}}{y_{ik}} \right) \leq 0, \quad i \in D_k, k \in K \quad (SP_n) \quad 409$$

$$410 \quad \sum_{i \in D_k} y_{ik} = 1, \quad k \in K \quad 410$$

$$411 \quad Ay \leq a \quad 411$$

$$412 \quad \beta_n^T x \leq b_n, \quad n = 1, 2, \dots, N \quad 412$$

$$413 \quad x, v_{ik} \in R^n, \quad 0 \leq y_{ik} \leq 1 \quad 413$$

414 Let the solution of the separation problem (SP_n) be
415 $x^{S,n}$. A cutting plane $\beta_n^T x \leq b_n$ can then be obtained
416 from:

$$417 \quad (x^{S,n} - x_R^{BM,n})^T (x - x^{S,n}) \geq 0 \quad (28) \quad 417$$

418 where the coefficient of x is a subgradient of the
419 objective function of (SP_n) at $x^{S,n}$ (for derivation, see
420 Stubbs & Mehrotra, 1999). Fig. 13 shows an example of
421 a cutting plane generated with the points $x^{S,n}$ and $x_R^{BM,n}$.

422 The cutting plane method can then be stated as
423 follows:

- 423 1) Solve continuous relaxation of (PC_n). 423
- 424 2) Solve separation problem (SP_n). 424
- 425 a) If $\|x^{S,n} - x_R^{BM,n}\| \leq \varepsilon$, stop. 425

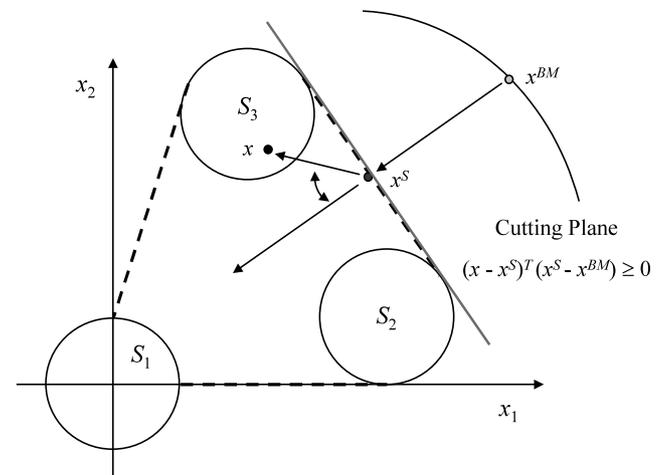


Fig. 13. Cutting plane generated by separation problem.

426 b) Else set $\beta_{n+1} = -(x^{S,n} - x_R^{BM,n})$ and $b_{n+1} =$
 427 $-(x^{S,n} - x_R^{BM,n})x^{S,n}$. Set $n = n+1$, return to
 428 Step 1.

429 This procedure can be used either in Branch and Cut
 430 enumeration method where a special case is to solve the
 431 separation problem only at the root node, or else it can
 432 be used to strengthen the MINLP model before apply-
 433 ing methods such as Outer-Approximation (OA), Gen-
 434 eralized Benders Decomposition (GBD), and Extended
 435 Cutting Plane (ECP). It is also interesting to note that
 436 cutting planes can be derived in the x - y space. In
 437 example 2, when we consider the cutting plane in the x
 438 space, the big-M relaxation solution, $x = (0.55, 0.55)$
 439 cannot be separated from the convex hull since it is
 440 feasible to the convex hull onto the x space. But when
 441 we consider the cutting plane in the x - y space, then the
 442 big-M relaxation solution, $(x, y) = (0.55, 0.55, 0.605)$
 443 can be separated from the convex hull since this point is
 444 infeasible to the convex hull relaxation Eq. (24). This
 445 suggests that the application of cutting planes in the x -
 446 y space may be more effective than in the x space only
 447 for cutting off the big-M relaxation point from the
 448 convex hull.

449 Another application of the separation problem is for
 450 deciding whether it is advantageous or not to use the
 451 convex hull formulation. If the value of $\|x^{S,n} - x_R^{BM,n}\|$ is
 452 large, then it is an indication that this is the case. A small
 453 difference between $x^{S,n}$ and $x_R^{BM,n}$ would indicate that it
 454 might be better to use the big-M relaxation.

455 It should be also noted that the proposed cutting
 456 plane method can be extended to nonconvex disjunctive
 457 constraints using the global optimization procedure by
 458 Lee and Grossmann (2001). In this method the non-
 459 convex constraints are replaced by convex under/over-
 460 estimators, with which the convex hull relaxation or big-
 461 M relaxation can be used. Therefore, one can use the
 462 cutting plane method to tighten the relaxation of the
 463 bounding convex constraints.

464 7. Disjunctive programming examples

465 In this section we present a number of examples to
 466 illustrate the application of the main concepts in this
 467 paper.

468 7.1. Example 3

470
$$\min Z = (x_1 - 6)^2 + (x_2 - 4)^2$$

s.t.

$$\begin{aligned} & \left[Y_1 \right. \\ & \left. (x_1 - 4)^2 + (x_2 - 2)^2 \leq 0.5 \right] \\ & \vee \left[Y_2 \right. \\ & \left. (x_1 - 3)^2 + (x_2 - 4)^2 \leq 1 \right] \\ & \vee \left[Y_3 \right. \\ & \left. (x_1 - 1)^2 + (x_2 - 1)^2 \leq 1.5 \right] \end{aligned}$$

$$0 \leq x_1, x_2 \leq 5 \quad (29)$$

The feasible region is shown in Fig. 14. Note that the
 471 point (6,4), which is the minimizer of the objective
 472 function, lies outside the convex hull of the disjunction.
 473 The optimal solution is $x = (4,4)$, $Z = 4.0$, $Y = (\text{false},$
 474 $\text{true}, \text{false})$.

To illustrate the cutting plane procedure, first we
 475 solve the big-M relaxation of Eq. (30) with $M = (19.5,$
 476 $24, 30.5)$ from Eq. (12). The solution is $x^{BM} = (5, 4)$,
 477 $Z^{BM} = 1.0$, $y^{BM} = (0.209, 0.561, 0.230)$. Then we solve
 478 the separation problem (SP_n) with the relaxation point
 479 $x^{BM} = (5, 4)$:
 480

$$\min Z = (x_1 - 5)^2 + (x_2 - 4)^2 \quad 481$$

$$\text{s.t. } x_1 = v_{11} + v_{12} + v_{13}$$

$$x_2 = v_{21} + v_{22} + v_{23}$$

$$(y_1 + \varepsilon) \left[\left(\frac{v_{11}}{y_1 + \varepsilon} - 4 \right)^2 + \left(\frac{v_{21}}{y_1 + \varepsilon} - 2 \right)^2 - 0.5 \right] \leq 0$$

$$(y_2 + \varepsilon) \left[\left(\frac{v_{12}}{y_2 + \varepsilon} - 3 \right)^2 + \left(\frac{v_{22}}{y_2 + \varepsilon} - 4 \right)^2 - 1 \right] \leq 0$$

$$(y_3 + \varepsilon) \left[\left(\frac{v_{13}}{y_3 + \varepsilon} - 1 \right)^2 + \left(\frac{v_{23}}{y_3 + \varepsilon} - 1 \right)^2 - 1.5 \right] \leq 0$$

$$y_1 + y_2 + y_3 = 1$$

$$0 \leq y_i \leq 1, \quad i = 1, 2, 3$$

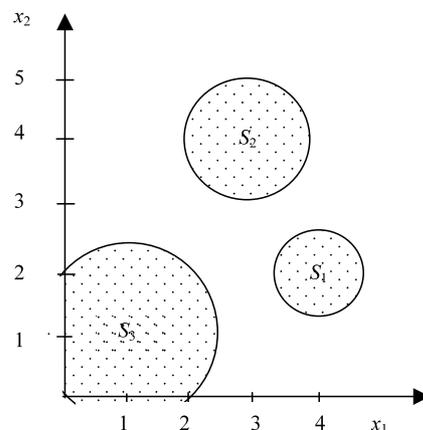


Fig. 14. Feasible region of example 3.

$$0 \leq v_{ji} \leq 5y_i \quad \forall i, \forall j$$

$$0 \leq x_1, x_2 \leq 5 \quad (30)$$

The solution of problem Eq. (31) is $x^S = (4.16, 3.70)$ with the objective value of 0.791. Therefore, the cutting plane is given as follows:

$$\begin{bmatrix} 4.16 - 5.0 \\ 3.70 - 4.0 \end{bmatrix}^T \begin{bmatrix} x_1 - 4.16 \\ x_2 - 3.70 \end{bmatrix} \geq 0 \quad (31)$$

which can be simplified as $-0.84(x_1 - 4.16) - 0.3(x_2 - 3.70) \geq 0$. We add Eq. (32) to the big-M relaxation and solve it again. The solution of this augmented big-M relaxation is $x^{CP} = (4.27, 3.4)$, $Z^{CP} = 3.37$, $y^{CP} = (0.294, 0.676, 0.029)$. For comparison, we solve the convex hull relaxation, obtaining $x^{CH} = (4.27, 3.4)$, $Z^{CH} = 3.37$, $y^{CH} = (0.442, 0.558, 0)$. Note that the solution x^{CP} and the objective value Z^{CP} are identical to x^{CH} and Z^{CH} . The difference in (x^{BM}, Z^{BM}) and (x^{CH}, Z^{CH}) is a clear indication that the convex hull is significantly tighter than big-M relaxation. For this example, only one cutting plane yields the same tightness of the relaxation as the convex hull. The numerical results are shown in Table 1. Note that the big-M relaxation yields the lowest objective value to the optimal solution, 4.0. Fig. 15 shows the convex hull and cutting plane. As shown in Fig. 15, the cutting plane is a facet of the convex hull. From Table 1 it can be seen that the big-M relaxation with a cutting plane yields a competitive relaxation compared with the convex hull.

7.2. Cutting planes in x - y space: example 2

Let us revisit example 2. If we apply the separation problem (SP_n) to the big-M relaxation solution $x_R^{BM} = (0.55, 0.55)$, the objective value of the separation problem is zero since x_R^{BM} is feasible to the convex hull relaxation of Eq. (23) in the x space. However, if we treat the binary variable y as continuous variable and then extend the dimension of the solution to the x - y space, we have the following separation problem with $(x, y)_R^{BM} = (0.55, 0.55, 0.605)$:

$$\begin{aligned} \min Z &= [(x_1 - 0.55)^2 + (x_2 - 0.55)^2 + (y_1 - 0.605)^2] \\ \text{s.t.} \\ x_1^2 + x_2^2 &\leq y_1^2 \end{aligned} \quad (\text{SP1})$$

Table 1
Comparisons of the relaxations for example 3

Relaxation	M	x_1	x_2	y_1	y_2	y_3	Z
Big-M	(19.5, 24, 30.5)	5.0	4.0	0.209	0.561	0.023	1.0
Convex hull	–	4.27	3.40	0.442	0.558	0.0	3.37
Cutting plane	–	4.27	3.40	0.294	0.676	0.029	3.37
Optimal solution	–	4.0	4.0	0	1	0	4.0

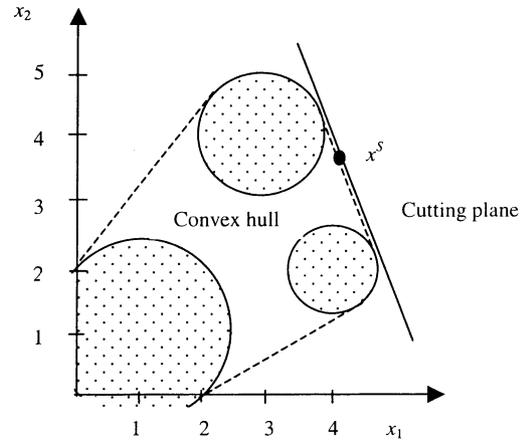


Fig. 15. Convex hull and cutting plane for example 3.

$$0 \leq x_1 \leq y_1 \quad 517$$

$$0 \leq x_2 \leq y_1 \quad 518$$

$$0 \leq y_1 \leq 1 \quad 519$$

The solution is $Z = 0.015$ and $(x, y)^S = (0.489, 0.489, 0.691)$, which means that $(x, y)_R^{BM}$ is infeasible in the convex hull relaxation Eq. (24) in the x - y space. The cutting plane is now given by $(0.489 - 0.55)(x_1 - 0.489) + (0.489 - 0.55)(x_2 - 0.489) + (0.691 - 0.605)(y_1 - 0.691) \geq 0$. When this cutting plane is added to the big-M relaxation Eq. (25), the optimal solution is $(x, y) = (0.707, 0.707, 1)$ and $Z = 1.309$, which is identical to the solution of the convex hull relaxation Eq. (24) and is also the optimal solution of Eq. (23). This shows that the cutting plane method applied to the x - y space can yield tighter relaxations than the cutting plane in the x space only.

7.3. Example 4

Consider the synthesis of a process network (Türky & Grossmann, 1996) where the following disjunctive set is used to model the problem:

$$\begin{bmatrix} Y_k \\ h_{ik}(x) = 0 \\ c_k = \gamma_k \end{bmatrix} \vee \begin{bmatrix} \neg Y_k \\ B_{ik}x = 0 \\ c_k = 0 \end{bmatrix} \quad i \in D_k, k \in K \quad (32) \quad 537$$

It means that if the k th unit is selected ($Y_k = \text{true}$) then the first term of the disjunction applies, if it is not ($\neg Y_k$) then a subset of the x variables is set to zero.

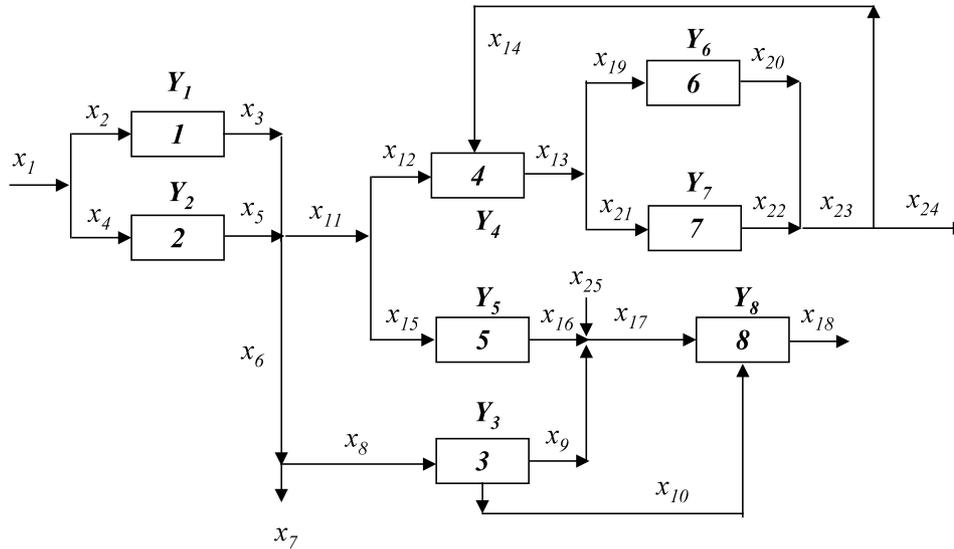


Fig. 16. Process superstructure of example 4.

540 Fig. 16 shows the superstructure of example 4, which
 541 has eight units. The corresponding GDP model is as
 542 follows:

$$543 \min Z = \sum_{k=1}^8 c_k + a^T x + 122$$

544 s.t. Mass balances:

$$545 x_1 = x_2 + x_4, \quad x_6 = x_7 + x_8$$

$$546 x_3 + x_5 = x_6 + x_{11}$$

$$547 x_{11} = x_{12} + x_{15}, \quad x_{13} = x_{19} + x_{21}$$

$$548 x_9 + x_{16} + x_{25} = x_{17}$$

$$549 x_{20} + x_{22} = x_{23}, \quad x_{23} = x_{14} + x_{24}$$

550 Specifications:

$$551 x_{10} - 0.8x_{17} \leq 0, \quad x_{10} - 0.4x_{17} \geq 0$$

$$552 x_{12} - 5x_{14} \leq 0, \quad x_{12} - 2x_{14} \geq 0$$

553 Disjuncts:

$$554 \left[\begin{array}{l} Y_1 \\ \exp(x_3) - 1 - x_2 \leq 0 \\ c_1 = 5 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_1 \\ x_3 = x_2 = 0 \\ c_1 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_2 \\ \exp\left(\frac{x_5}{1.2}\right) - 1 - x_4 \leq 0 \\ c_2 = 5 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_2 \\ x_4 = x_5 = 0 \\ c_2 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_3 \\ 1.5x_9 + x_{10} - x_8 = 0 \\ c_3 = 6 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_3 \\ x_9 = 0, \quad x_8 = x_{10} \\ c_3 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_4 \\ 1.25(x_{12} + x_{14}) - x_{13} = 0 \\ c_4 = 10 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_4 \\ x_{12} = x_{13} = x_{14} = 0 \\ c_4 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_5 \\ x_{15} - 2x_{16} = 0 \\ c_5 = 6 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_5 \\ x_{15} = x_{16} = 0 \\ c_5 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_6 \\ \exp\left(\frac{x_{20}}{1.5}\right) - 1 - x_{19} \leq 0 \\ c_6 = 7 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_6 \\ x_{19} = x_{20} = 0 \\ c_6 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_7 \\ \exp(x_{22}) - 1 - x_{21} \leq 0 \\ c_7 = 4 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_7 \\ x_{21} = x_{22} = 0 \\ c_7 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_8 \\ \exp(x_{18}) - 1 - x_{10} - x_{17} \leq 0 \\ c_8 = 5 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_8 \\ x_{10} = x_{17} = x_{18} = 0 \\ c_8 = 0 \end{array} \right] \quad (33)$$

Logic propositions:

$$Y_1 \Rightarrow Y_3 \vee Y_4 \vee Y_5 \quad Y_5 \Rightarrow Y_8 \quad 556$$

$$Y_2 \Rightarrow Y_3 \vee Y_4 \vee Y_5 \quad Y_6 \Rightarrow Y_4 \quad 557$$

$$Y_3 \Rightarrow Y_1 \vee Y_2 \quad Y_7 \Rightarrow Y_4 \quad 558$$

$$Y_3 \Rightarrow Y_8 \quad Y_8 \Rightarrow Y_3 \vee Y_5 \vee (\neg Y_3 \wedge \neg Y_5) \quad 559$$

$$Y_4 \Rightarrow Y_1 \vee Y_2 \quad Y_1 \perp Y_2 \quad 560$$

$$Y_4 \Rightarrow Y_6 \vee Y_7 \quad Y_4 \perp Y_5 \quad 561$$

$$Y_5 \Rightarrow Y_1 \vee Y_2 \quad Y_6 \perp Y_7 \quad 562$$

Problem data: 563

$$a^T = (a_1 = 0, a_2 = 10, a_3 = 1, a_4 = 1, a_5 = -15, a_6 = 0, \quad 564$$

$$a_7 = 0, a_8 = 0, a_9 = -40, a_{10} = 15, a_{11} = 0, a_{12} = 0, a_{13} = \quad 565$$

$$0, a_{14} = 15, a_{15} = 0, a_{16} = 0, a_{17} = 80, a_{18} = -65, a_{19} = \quad 566$$

567 25, $a_{20} = -60$, $a_{21} = 35$, $a_{22} = -80$, $a_{23} = 0$, $a_{24} = 0$,
568 $a_{25} = -35$); $x_j^{\text{lo}} = 0$, $\forall j$.

569 Before introducing the big-M relaxation, it should be
570 noted that in the disjunctions we have the following
571 properties:

- 572 i) The disjunctions are *improper* since the feasible
573 region of the second term belongs to the feasible
574 region of the first term in x space (except the cost
575 term).
576 ii) In the second term of the disjunctions a subset of
577 the continuous variables x are zero.
578 iii) No continuous variable x is repeated in the second
579 term ($\neg Y_k$) of the disjunctions.

580 Because of these properties, it is possible to rewrite the
581 disjunctions as follows:

582 $\exp(x_3) - 1 - x_2 \leq 0$

583 $\exp\left(\frac{x_5}{1.2}\right) - 1 - x_4 \leq 0$

584 $1.5x_9 + x_{10} - x_8 = 0$

585 $1.25(x_{12} + x_{14}) - x_{13} = 0$

586 $x_{15} - 2x_{16} = 0$

587 $\exp\left(\frac{x_{20}}{1.5}\right) - 1 - x_{19} \leq 0$

588 $\exp(x_{22}) - 1 - x_{21} \leq 0$

589 $\exp\left(\frac{x_{18}}{1.5}\right) - 1 - x_{10} - x_{17} \leq 0$

590 Disjunctions:

591
$$\begin{bmatrix} Y_1 \\ 0 \leq x_2 \leq x_2^{\text{up}} \\ 0 \leq x_3 \leq x_3^{\text{up}} \\ c_1 = 5 \end{bmatrix} \vee \begin{bmatrix} \neg Y_1 \\ x_3 = x_2 = 0 \\ c_1 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_2 \\ 0 \leq x_4 \leq x_4^{\text{up}} \\ 0 \leq x_5 \leq x_5^{\text{up}} \\ c_2 = 5 \end{bmatrix} \vee \begin{bmatrix} \neg Y_2 \\ x_4 = x_5 = 0 \\ c_2 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_3 \\ 0 \leq x_9 \leq x_9^{\text{up}} \\ c_3 = 6 \end{bmatrix} \vee \begin{bmatrix} \neg Y_3 \\ x_9 = 0 \\ c_3 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_4 \\ 0 \leq x_{12} \leq x_{12}^{\text{up}} \\ 0 \leq x_{13} \leq x_{13}^{\text{up}} \\ 0 \leq x_{14} \leq x_{14}^{\text{up}} \\ c_4 = 10 \end{bmatrix} \vee \begin{bmatrix} \neg Y_4 \\ x_{12} = x_{13} = x_{14} = 0 \\ c_4 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_5 \\ 0 \leq x_{15} \leq x_{15}^{\text{up}} \\ 0 \leq x_{16} \leq x_{16}^{\text{up}} \\ c_5 = 6 \end{bmatrix} \vee \begin{bmatrix} \neg Y_5 \\ x_{15} = x_{16} = 0 \\ c_5 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_6 \\ 0 \leq x_{19} \leq x_{19}^{\text{up}} \\ 0 \leq x_{20} \leq x_{20}^{\text{up}} \\ c_6 = 7 \end{bmatrix} \vee \begin{bmatrix} \neg Y_6 \\ x_{19} = x_{20} = 0 \\ c_6 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_7 \\ 0 \leq x_{21} \leq x_{21}^{\text{up}} \\ 0 \leq x_{22} \leq x_{22}^{\text{up}} \\ c_7 = 4 \end{bmatrix} \vee \begin{bmatrix} \neg Y_7 \\ x_{21} = x_{22} = 0 \\ c_7 = 0 \end{bmatrix}$$

$$\begin{bmatrix} Y_8 \\ 0 \leq x_{10} \leq x_{12}^{\text{up}} \\ 0 \leq x_{17} \leq x_{13}^{\text{up}} \\ 0 \leq x_{18} \leq x_{14}^{\text{up}} \\ c_8 = 5 \end{bmatrix} \vee \begin{bmatrix} \neg Y_8 \\ x_{10} = x_{17} = x_{18} = 0 \\ c_8 = 0 \end{bmatrix} \quad (34)$$

592 It should be noted that constraints Eq. (35) consist of
593 global constraints (nonlinear) and disjunctions (linear).
594 The convex hull of the above disjunctions can be
595 reduced to linear constraints for the big-M relaxation

$$0 \leq x_j \leq x_j^{\text{up}} y_k, \quad j \in J, \quad k \in K \quad (35) \quad 596$$

$$c_k = \gamma_k y_k, \quad k \in K \quad 597$$

$$0 \leq y_k \leq 1, \quad k \in K \quad 598$$

599 which means that if the first term of the disjunction is
600 true ($y_k = 1$) then the continuous variables x_j can have
601 a value between its bounds and the fixed cost is activated,
602 else if the second term is true ($y_k = 0$) then the
603 continuous variables become zero that still satisfies the
604 global constraints (condition i).

605 The GDP problem Eq. (34) is solved with the convex
606 hull relaxation. The upper bounds used are $x_3^{\text{up}} = 2$,
607 $x_5^{\text{up}} = 2$, $x_9^{\text{up}} = 2$, $x_{10}^{\text{up}} = 1$, $x_{17}^{\text{up}} = 1$, $x_{19}^{\text{up}} = 2$, $x_{21}^{\text{up}} = 2$,
608 $x_{22}^{\text{up}} = 3$, and for the rest of the variables, $x_j^{\text{up}} = 6.5$.
609 The objective function value $Z = 64.8$ was obtained
610 from the convex hull relaxation, and the corresponding
611 NLP requires 0.07 CPU s with CONOPT/GAMS.
612 Applying the big-M relaxation to the modified GDP
613 formulation Eq. (35) and the same bounds, we obtained
614 $Z = 49.9$ as the solution value. Therefore, the convex
615 hull relaxation of the original GDP model yields a much
616 tighter lower bound. The difference between these two
617 relaxation values comes from the fact that the feasible
618 region by the convex hull relaxation of nonlinear
619 disjunctions Eq. (34) in the x - y space is tighter than
620 the feasible region by big-M relaxation of Eq. (35).
621 However, it should be noted that their projections onto
622 the x space are identical since the disjunctions are
623 *improper*. If the disjunctions are linear, then both

relaxations can be identical in the x - y space if appropriate big-M parameters are used.

Since the convex hull relaxation yields a significant increase in the number of additional constraints and variables, we consider the generation of cutting planes to strengthen the big-M relaxation. As outlined in Section 6, a separation problem is solved. And the solution of the separation problem is used to build a cutting plane as in example 4. The big-M relaxation of Eq. (35) is then solved again with this cutting plane. Since the cutting plane is a facet of the convex hull, it will tighten the lower bound. Table 2 shows the increase of the lower bound as cutting planes are added to the big-M relaxation. The first column shows the number of cutting planes added. The second column shows the relaxation value. Note that the optimal solution of example 4 is 68.01. The third column shows the objective value of the separation problem. As more cutting planes are added, the objective value of the separation problem decreases, implying that the solution point of the augmented big-M relaxation gets closer to the convex hull. The fourth column shows the CPU time of separation problem. The fifth and sixth column show the MINLP solution results by DICOPT++ with the corresponding cuts. In all cases, the optimal solution is found in the second major iteration. Since this problem is a convex MINLP, the Outer-Approximation (OA) algorithm stops when the crossover occurs. The CPU time is less than 1 s on a Pentium III PC 600 MHz with 128 Mbytes RAM memory. After adding seven cutting planes, the lower bound improved significantly compared with the case when no cutting plane is used (62.5 vs. 49.9). The advantage of the cutting plane method is that only one linear constraint is added to the big-M relaxation at each step. However, there is a cost for building a cutting plane and that is to solve a separation problem, which is a convex NLP problem (SP_n).

7.4. Example 5

To illustrate the application of the cutting plane method with a branch and bound algorithm, we have constructed the following GDP problem with linear/

nonlinear *proper* disjunctions.

$$\min Z = \sum_{k=1}^9 c_k + a^T x \quad 666$$

$$-0.6 \log(x_{12} + 1) + 0.8(x_{13} - 8)^2 + 0.7 \exp(-x_{14} + 1) - 0.5 \log(x_{15} + 2) \quad 667$$

s.t. Mass balances: 668

$$x_1 = x_5 + x_6, \quad x_4 = x_7 + x_8 \quad 669$$

$$x_{10} = x_{19} + x_{20}, \quad x_{11} = x_{17} + x_{18} \quad 670$$

$$x_{14} = x_{21} + x_{22}, \quad x_9 = x_{23} + x_{24} \quad 671$$

$$x_{12} = x_{25} + x_{26} \quad 672$$

Specifications: 673

$$x_1 + x_2 + x_3 + x_4 \leq 30 \quad 674$$

$$x_9 + x_{10} + x_{11} \leq 25 \quad 675$$

$$x_{12} + x_{13} + x_{14} + x_{15} + x_{16} \leq 20 \quad 676$$

$$\left[\begin{array}{l} Y_1 \\ x_9 \leq 1.7 \log(x_2 + x_5 + 1) \\ x_9 \geq 0.1 + 0.2x_5 \\ x_5 \geq 2x_2 \\ c_1 = 2 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_1 \\ x_2 = x_5 = x_9 = 0 \\ c_1 = 0 \end{array} \right] \quad 677$$

$$\left[\begin{array}{l} Y_2 \\ x_{10} = 0.9x_3 + 0.8x_7 \\ 1 \leq x_3 + x_7 \\ x_7 \geq x_3 \\ c_2 = 1 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_2 \\ x_3 = x_7 = x_{10} = 0 \\ c_2 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_3 \\ 1.5x_{11} = x_6 + x_8 \\ x_6 = x_8 \\ x_{11} \geq 1 \\ c_3 = 9 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_3 \\ x_6 = x_8 = x_{11} = 0 \\ c_3 = 0 \end{array} \right]$$

$$\left[\begin{array}{l} Y_4 \\ x_{25} \leq \log(x_{23} + 1) + 0.1 \\ x_{25} \geq 1 \\ c_4 = 1.5 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_4 \\ x_{23} = x_{25} = 0 \\ c_4 = 0 \end{array} \right]$$

Table 2
Numerical results of cutting plane method for example 4

Number of cutting planes	Big-M relaxation	Separation problem solution	Separation CPU (s)	DICOPT++ major iterations	GPU (s)
0	49.9	0.545	0.043	2	0.139
1	51.7	0.701	0.078	2	0.129
2	52.2	0.576	0.078	2	0.121
3	53.2	0.163	0.027	2	0.139
4	61.2	0.010	0.039	2	0.248
5	61.9	0.004	0.051	2	0.151
6	62.4	0.005	0.051	2	0.143
7	62.5	0.002	0.051	2	0.157

$$\begin{aligned}
& \left[\begin{array}{l} Y_5 \\ x_{26} \leq 1.5 \log(x_{24} + 1) \\ x_{26} \geq 1 \\ c_5 = 4 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_5 \\ x_{24} = x_{26} = 0 \\ c_5 = 0 \end{array} \right] \\
& \left[\begin{array}{l} Y_6 \\ (x_{17} - 4)^2 + (x_{21} - 4)^2 \leq 12 \\ x_{21} \geq 1 \\ c_6 = 3.7 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_6 \\ x_{17} = x_{21} = 0 \\ c_6 = 0 \end{array} \right] \\
& \left[\begin{array}{l} Y_7 \\ x_{13} \leq 7 - 1.2(x_{20} - 3)^2 \\ x_{22} \leq 8 - (x_{20} - 3)^2 \\ x_{20} \geq 1 \\ c_7 = 7.4 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_7 \\ x_{13} = x_{20} = x_{22} = 0 \\ c_7 = 0 \end{array} \right] \\
& \left[\begin{array}{l} Y_8 \\ x_{15} \leq 1.2 \log(x_{19} + 2) \\ x_{15} \geq 1 + 0.2x_{19} \\ x_{19} \geq 1 \\ c_8 = 6.5 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_8 \\ x_{15} = x_{19} = 0 \\ c_8 = 0 \end{array} \right] \\
& \left[\begin{array}{l} Y_9 \\ x_{16} + x_{18} \geq 5 \\ x_{16} \leq 6 + 2 \log(x_{18} + 1) \\ x_{18} \geq 1 \\ c_9 = 5.2 \end{array} \right] \vee \left[\begin{array}{l} \neg Y_9 \\ x_{16} = x_{18} = 0 \\ c_9 = 0 \end{array} \right] \quad (36)
\end{aligned}$$

Logic proposition:

$$\begin{aligned}
678 & Y_1 \vee Y_2 \vee Y_3 \\
679 & \neg(Y_1 \wedge Y_2 \wedge Y_3) \\
680 & \neg Y_4 \vee \neg Y_5 \\
681 & Y_1 \Rightarrow Y_4 \vee Y_5 \\
682 & Y_4 \Rightarrow Y_1 \\
683 & Y_5 \Rightarrow Y_1 \\
684 & Y_2 \Rightarrow Y_7 \vee Y_8 \\
685 & Y_3 \Rightarrow Y_6 \vee Y_9 \\
686 & Y_6 \Rightarrow Y_3 \\
687 & \neg Y_8 \vee \neg Y_9 \\
688 & Y_9 \Rightarrow Y_3 \\
689 & [Y_4 \vee Y_5] \Rightarrow [Y_7 \vee Y_8 \vee Y_9] \\
690 & [\neg Y_4 \wedge \neg Y_5] \Rightarrow [Y_7 \wedge Y_8] \vee [Y_8 \wedge Y_9] \vee [Y_7 \wedge Y_9] \\
691 & 0 \leq x_j \leq 9 \quad j = 1, \dots, 26; \quad 0 \leq c_k, \quad Y_k \in \{\text{true}, \text{false}\}, \\
& \quad k = 1, \dots, 9
\end{aligned}$$

692 The optimal solution is $Z = -197.3$,
693 $Y_2, Y_3, Y_6, Y_7, Y_9 = \text{true}$ and $x = (1.15, 0, 1.56, 2.72, 0,$
694 $1.15, 1.56, 1.15, 0, 2.67, 1.53, 0, 6.87, 9, 0, 7.38, 0.53, 1, 0, 2.67,$
695 $4.02, 4.98, 0, 0, 0, 0)$. The big-M relaxation of Eq. (36)
696 yields a lower bound of -326.4 . The convex hull
697 relaxation of problem Eq. (36) yields a lower bound of
698 -209 . Table 3 shows the results of cutting plane method
699 applied to big-M relaxation of Eq. (36). As more cutting
700 planes are added, the lower bound of big-M relaxation

Table 3
Numerical results of cutting plane method for example 5

Number of cutting planes	Big-M relaxation solution	Separation problem solution
0	-326.4	91.2
1	-265.6	5.97
2	-255.8	9.76
3	-245.5	7.12
4	-239.5	4.34
5	-238.0	4.35
6	-224.4	2.39
7	-223.4	1.31
8	-221.4	0.91
9	-220.8	0.25
10	-219.7	0.19
Convex hull relaxation	-209.0	0

increases and the objective value of the separation
701 problem decreases. After adding ten cutting planes, the
702 lower bound significantly improved (-219.7). Table 4
703 shows the branch and bound search results when cutting
704 planes are added before starting the branch and bound
705 search. First, the big-M MINLP problem is solved with
706 branch and bound search. Nineteen nodes are searched
707 and the optimal solution -197.3 is found. Secondly,
708 four cutting planes are added to big-M MINLP problem
709 at the root node of branch and bound tree. Note that the
710 relaxation value, which is the objective value at the root
711 node, is -239.5 and 13 nodes are searched to find the
712 optimal solution. The decrease in the number of search
713 nodes is due to the tighter relaxation value. When eight
714 cutting planes are added, the relaxation value is -221.4
715 and only seven nodes are searched. For comparison, the
716 convex hull relaxation of Eq. (36) is solved and the
717 number of nodes is seven, which is same as in the case of
718 eight cutting planes. The CPU time for each case is also
719 shown in Table 4 and less CPU time is spent with fewer
720 number of nodes. The CPU time for generating eight
721 cutting planes is about 2 s. This example clearly shows
722 that the cutting planes can tighten the relaxation and
723 thus reduce the number of search nodes in branch and
724 bound method. Although the example presented is
725 rather small, the proposed cutting plane method should
726 be promising for solving larger problems. This will be
727 the subject of our future work. 728

8. Conclusions 729

The purpose of this paper has been to analyze the
730 different alternatives of modeling the discrete choices as
731 disjunctions or as mixed-integer (0–1) inequalities, in
732 order to provide guidelines on this decision. The
733 resulting model can correspond to one of the three
734 formulations: mixed-integer constraints (PA), disjunc-
735 tive constraints (GDP) or hybrid (PH). For the analysis,
736

Table 4
Comparisons of branch and bound search results for example 5

Model	Big-M MINLP no cutting planes	Big-M MINLP +4 cutting planes	Big-M MINLP +8 cutting planes	Convex hull relaxation
Relaxation value	−326.4	−239.5	−221.4	−209.0
Optimal solution	−197.3	−197.3	−197.3	−197.3
Number of nodes	19	13	7	7
CPU s	3.39	2.53 ^a	1.56 ^a	1.62

^a CPU time for generating cutting planes is not included.

we considered three different possible relaxations of a disjunctive set, the convex hull, the big-M relaxation and the Beaumont surrogate. The analysis was performed mainly on the first two since the big-M formulation is widely used.

Although it was proved that the convex hull relaxation yields a tighter relaxation than the traditional 0–1 big-M relaxation, there are several cases when the big-M relaxation can compete with the convex hull relaxation. As a general rule, the big-M model is competitive when good bounds can be provided for the variables, and for large problems where it is important to keep the number of equations and variables as small as possible. For convex *improper* disjunction both the convex hull and the big-M model give the same relaxation in the x space, but this may not be true in the x – y space as was demonstrated with examples. For *proper* disjunctions where the feasible regions have some intersection, the objective function plays an important role, if the minimizer of the objective function is inside the feasible region of the disjunctive set, both the big-M and the convex hull relaxation may yield the same relaxation value. Otherwise the convex hull should be generally better, but the big-M constraints with appropriate bounds can be competitive. For *proper* disjunctions with an empty intersection on the feasible regions (disjoint terms) the convex hull is generally better than the big-M relaxation. Although these conclusions are not general, we believe they help to provide some insight in the modeling of discrete/continuous optimization problems.

Finally, to address the problem of formulating tight models without generating the explicit equations of the convex hull, a cutting plane algorithm has been proposed. A number of examples have been presented to illustrate the various ideas in this paper as well as the cutting plane method.

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Appendix A: Property of relaxations

Property 1. Let R_{BM} be the feasible set of big-M relaxation of a given disjunctive set projected onto the x space. Let R_{CH} be the feasible set of convex hull relaxation projected onto the x space. Let R_B be the feasible set of the Beaumont surrogate that is defined in the x space. Then $R_{CH} \subseteq R_{BM} \subseteq R_B$.

Proof. First consider $R_{BM} \subseteq R_B$. For the linear case, Beaumont (1990) proved that $R_{BM} = R_B$. Therefore, $R_{BM} \subseteq R_B$ holds. For the nonlinear case, we consider one disjunction for simplicity. Given a nonlinear disjunctive set:

$$F = \bigvee_{i \in D} [h_i(x) \leq 0] \quad x \in R^n \quad (A1)$$

where $h_i(x)$ are assumed to be convex bounded functions. The big-M relaxation of Eq. (A1) is as follows:

$$\sum_{i \in D} y_i = 1 \quad (A3)$$

$$0 \leq y_i \leq 1, \quad i \in D \quad (A4)$$

where $M_i = \max\{h_i(x) | x^L \leq x \leq x^U\}$. Let $R_{BM}^F(x, y)$ be the feasible set defined by Eqs. (A2), (A3) and (A4). The Beaumont surrogate of Eq. (A1) is given by:

$$\sum_{i \in D} \frac{h_i(x)}{M_i} \leq N - 1 \quad (A5)$$

where $N = |D|$ and M_i are assumed to be same as in Eq. (A2). Let $R_B^F(x, y)$ be the feasible set defined by Eqs. (A5) and (A4). Since Eq. (A5) is given by a linear combination of Eqs. (A2) and (A3), any feasible point $(x^*, y^*) \in R_{BM}^F(x, y)$ also satisfies Eqs. (A5) and (A4). Hence, $(x^*, y^*) \in R_B^F(x, y)$. Therefore, $R_{BM}^F(x, y) \subseteq R_B^F(x, y)$. Since R_{BM} and R_B are the projection of $R_{BM}^F(x, y)$ and $R_B^F(x, y)$ onto the x space, it follows that:

$$R_{BM} \subseteq R_B \quad (A6)$$

Secondly, we consider $R_{CH} \subseteq R_{BM}$ for linear and nonlinear case. The convex hull relaxation of Eq. (A1) is given by:

$$x - \sum_{i \in D} v_i = 0 \quad x, v_i \in R^n \quad (A7)$$

$$809 \quad y_i h_i \left(\frac{v_i}{y_i} \right) \leq 0, \quad i \in D \quad (\text{A8})$$

$$810 \quad \sum_{i \in D} y_i = 1 \quad (\text{A9})$$

$$811 \quad 0 \leq y_i \leq 1, \quad i \in D \quad (\text{A10})$$

$$812 \quad 0 \leq v_i \leq v_i^U y_i, \quad i \in D \quad (\text{A11})$$

813 Let $R_{\text{CH}}^{\text{F}}(x, y, v)$ be the feasible set defined by Eqs.
814 (A7), (A8), (A9), (A10) and (A11). Consider any feasible
815 point $(x^*, y^*, v^*) \in R_{\text{CH}}^{\text{F}}(x, y, v)$. From Eq. (A7), there
816 exist μ_i such that:

$$817 \quad y_i \mu_i = v_i, \quad i \in D \quad (\text{A12})$$

$$818 \quad h_i(\mu_i) \leq 0, \quad i \in D \quad (\text{A13})$$

819 Since $h_i(x)$ are convex functions, for any $l \in D$:

$$820 \quad h_l(x) = h_l \left(\sum_{i \in D} y_i \mu_i \right) \leq \sum_{i \in D} y_i h_l(\mu_i) \quad (\text{A14})$$

821 For $h_l(\mu_i) \leq 0$ and $h_l(\mu_i)_{i \neq l} \leq M_l$, it follows from
822 Eqs. (A14), (A10) and (A11):

$$823 \quad h_l(x) \leq \sum_{i \in D, i \neq l} y_i M_l = M_l(1 - y_l) \quad (\text{A15})$$

824 Eq. (A15) is identical to Eq. (A2) in the big-M
825 relaxation for $l \in D$. Hence, any feasible point $(x^*, y^*, v^*) \in R_{\text{CH}}^{\text{F}}(x, y, v)$ has a corresponding feasible point
826 (x^*, y^*) which satisfies Eqs. (A2), (A3) and (A4).
827 Therefore, $(x^*, y^*) \in R_{\text{BM}}^{\text{F}}(x, y)$. Since R_{BM} and R_{CH}
828 are the projection of $R_{\text{BM}}^{\text{F}}(x, y)$ and $R_{\text{CH}}^{\text{F}}(x, y, v)$ onto
829 the x space, it follows that:

$$831 \quad R_{\text{CH}} \subseteq R_{\text{BM}} \quad (\text{A16})$$

832 From Eqs. (A6) and (A16), $R_{\text{CH}} \subseteq R_{\text{BM}} \subseteq R_{\text{B}}$. This
833 completes the proof.
882

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