Generalized disjunctive programming: A framework for formulation and alternative algorithms for MINLP optimization

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Mixed-Integer Nonlinear Optimization: Algorithmic Advances and Applications
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Motivation

- Discrete/Continuous Optimization
  - Nonlinear models
  - 0-1 and continuous decisions

- Optimization Models
  - Mixed-Integer Linear Programming (MILP)
  - Mixed-Integer Nonlinear Programming (MINLP)

Alternative approach:

- Logic-based: Generalized Disjunctive Programming (GDP)

- Challenges
  - How to develop "best" model?
  - How to improve relaxation?
  - How to solve nonconvex GDP problems to global optimality?

Outline

1. **Overview of major relaxations for nonlinear GDP and algorithms**

2. **Linear GDP: hierarchy of relaxations**

3. **Global Optimization of nonconvex GDP**

Ph.D. Students
Ramesh Raman
Metin Turkay
Sangbum Lee
Nick Sawaya
Juan Ruiz

MINLP

- **Mixed-Integer Nonlinear Programming**

$$\min Z = f(x, y) \qquad \textit{Objective Function}$$

$$s.t. \quad g(x, y) \le 0 \qquad \textit{Inequality Constraints}$$

$$x \in X,\ y \in Y$$

$$X = \{x \mid x \in R^n, x^L \le x \le x^U, Bx \le b\}$$

$$Y = \{y \mid y \in \{0,1\}^m, Ay \le a\}$$

- ***f(x,y)*** **and** ***g(x,y)*** **- assumed to be convex and bounded over X.**
- ***f(x,y)*** **and** ***g(x,y)*** **commonly linear in y**

Mixed-integer Nonlinear Programming

Algorithms

Branch and Bound (BB) *Ravindran and Gupta (1985), Stubbs, Mehrotra (1999), Leyffer (2001)*

Generalized Benders Decomposition (GBD) *Geoffrion (1972)*

Outer-Approximation (OA) *Duran and Grossmann (1986), Fletcher and Leyffer (1994)*

LP/NLP based Branch and Bound *Quesada, Grossmann (1994)*

Extended Cutting Plane(ECP) *Westerlund and Pettersson (1992)*

Codes:

SBB *GAMS simple B&B*

MINLP-BB (AMPL)*Fletcher and Leyffer (1999)*

Bonmin (COIN-OR) *Bonami et al (2006)*

FilMINT *Linderoth and Leyffer (2006)*

DICOPT (GAMS) *Viswanathan and Grossman (1990)*

AOA (AIMSS*)*

α–ECP *Westerlund and Peterssson (1996)*

MINOPT *Schweiger and Floudas (1998)*

BARON *Sahinidis et al. (1998)*

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Generalized Disjunctive Programming

Motivation

1. Facilitate modeling of discrete/continuous optimization problems through use algebraic constraints and symbolic expressions
2. Reduce combinatorial search effort
3. Improve handling nonlinearities

Generalized Disjunctive Programming (GDP)

- Raman and Grossmann (1994)   *(Extension Balas, 1979)*

$$\min \quad Z = \sum_k c_k + f(x)$$ **Objective Function**

$$s.t. \quad r(x) \le 0$$ **Common Constraints**

OR operator ⟶
$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix}, k \in K$$

Disjunction

Constraints

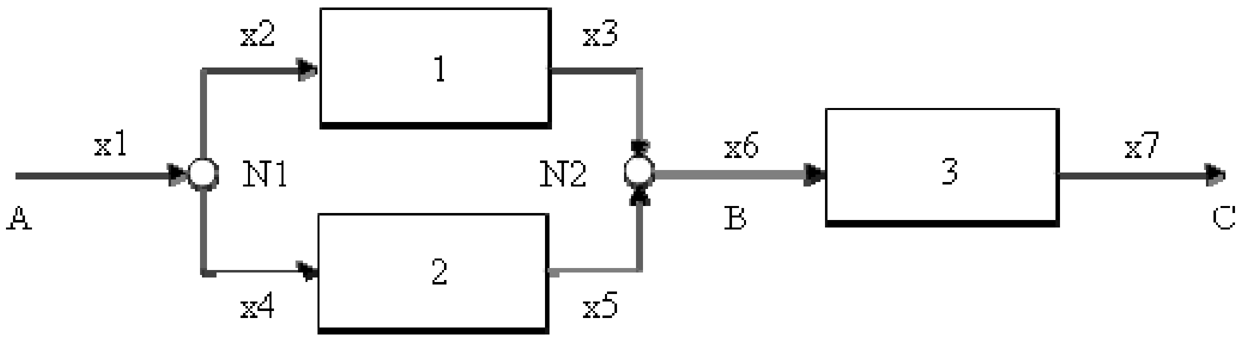
Fixed Charges

$$\Omega(Y) = true$$ **Logic Propositions**

$$x \in R^n, c_k \in R^1$$ **Continuous Variables**

$$Y_{jk} \in \{ true, \ false \}$$ **Boolean Variables**

Process Network with fixed charges



GDP model

$$
\begin{aligned}
&Min\ Z = c_1 + c_2 + c_3 + d^T x \\
&s.t. \\
&x_1 = x_2 + x_4 \\
&x_6 = x_3 + x_5 \\
&\begin{bmatrix} Y_{11} \\ x_3 = p_1 x_2 \\ c_1 = \gamma_1 \end{bmatrix} \vee \begin{bmatrix} Y_{21} \\ x_3 = x_2 = 0 \\ c_1 = 0 \end{bmatrix} \\
&\begin{bmatrix} Y_{12} \\ x_5 = p_2 x_4 \\ c_2 = \gamma_2 \end{bmatrix} \vee \begin{bmatrix} Y_{22} \\ x_5 = x_4 = 0 \\ c_2 = 0 \end{bmatrix} \\
&\begin{bmatrix} Y_{13} \\ x_7 = p_3 x_6 \\ c_3 = \gamma_3 \end{bmatrix} \vee \begin{bmatrix} Y_{23} \\ x_7 = x_6 = 0 \\ c_3 = 0 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&Y_{11} \underline{\vee}\, Y_{21} \\
&Y_{12} \underline{\vee}\, Y_{22} \\
&Y_{13} \underline{\vee}\, Y_{23} \\
&Y_{11} \vee Y_{12} \Rightarrow Y_{13} \\
&Y_{13} \Rightarrow Y_{11} \vee Y_{12} \\
&Y_{21} \vee Y_{22} \\
&0 \le x \le x^U \\
&Y_{11}, Y_{21}, Y_{12}, Y_{22}, Y_{13}, Y_{23} \in \{True, False\} \\
&c_1, c_2, c_3 \in \mathbb{R}^1
\end{aligned}
$$

Generalized Disjunctive Programming (GDP)

- Raman and Grossmann (1994)

	$\min \ Z = \sum_k c_k + f(x)$	**Objective Function**
	$s.t. \quad r(x) \le 0$	**Common Constraints**
OR operator ⟶	$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix}, k \in K$	**Disjunction** **Constraints** **Fixed Charges**
	$\Omega(Y) = true$	**Logic Propositions**
	$x \in R^n, c_k \in R^1$	**Continuous Variables**
	$Y_{jk} \in \{true, \ false\}$	**Boolean Variables**

Relaxation?

Big-M MINLP (BM)

- **MINLP reformulation of GDP**

$$
\begin{aligned}
\min Z \;&= \sum_{k\in K}\sum_{j\in J_k}\gamma_{jk}\lambda_{jk} + f(x)\\
s.t.\quad & r(x)\le 0\\
& g_{jk}(x)\le M_{jk}(1-\lambda_{jk})\quad ,j\in J_k, k\in K\\
& \sum_{j\in J_k}\lambda_{jk}=1,\;\; k\in K\\
& A\lambda\le a\\
& x\ge 0, \lambda_{jk}\in\{0,1\}
\end{aligned}
$$

Big-M Parameter

Logic constraints

NLP Relaxation $\quad 0\le \lambda_{jk}\le 1$

Convex Hull Formulation

- **Consider Disjunction $k \in K$**

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c = \gamma_{jk} \end{bmatrix}$$

- **Theorem: Convex Hull of Disjunction k** ***(Lee, Grossmann, 2000)***
  - **Disaggregated variables ν^j**

$$\{(x,c) \mid x = \sum_{j \in J_k} v^{jk}, \quad c_k = \sum_{j \in J} \lambda_{jk} \gamma_{jk},$$

$$0 \le v^{jk} \le \lambda_{jk} U_{jk}, \; j \in J_k$$

=> Convex Constraints

$$\sum_{j \in J_k} \lambda_{jk} = 1, \quad 0 < \lambda_{jk} \le 1,$$

$$\lambda_{jk} g_{jk}(v^{jk} / \lambda_{jk}) \le 0, \; j \in J_k \}$$

  - **λ_j - weights for linear combination**

- Generalization of Balas (1979)

Stubbs and Mehrotra (1999)

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Remarks

1. $\boldsymbol{h(\nu\ ,\lambda) = \lambda\, g\ (\nu\ \ /\lambda)}$

   If g(x) is a bounded convex function,

   $\boldsymbol{h(\nu\ ,\lambda)}$ is a bounded convex function

   Hiriart-Urruty and Lemaréchal (1993)

   $\boldsymbol{h(\nu,0) = 0}$ for bounded g(x)

2. Replace $\lambda_{jk} g_{jk}(\nu_{jk} / \lambda_{jk}) \leq 0$ where $0 \leq \nu_{jk} \leq U \lambda_{jk}$ by:

$$\boxed{((1-\varepsilon)\lambda_{jk} + \varepsilon)(g_{jk}(\nu_{jk} / ((1-\varepsilon)\lambda_{jk} + \varepsilon))) - \varepsilon g_{jk}(0)(1-\lambda_{jk}) \leq 0}$$

Furman, Sawaya & Grossmann (2007)

a. Exact approximation of the original constraints as $\varepsilon \to 0$.

b. The constraints are exact at $\lambda_{jk} = 0$ and at $\lambda_{jk} = 1$ regardless of value of ε.

$$if\ \lambda_{jk} = 0,\ \Rightarrow\ (\varepsilon)(g_{jk}(0)) - \varepsilon g_{jk}(0) = 0 \leq 0$$

$$if\ \lambda_{jk} = 1, \Rightarrow\ ((1)(g_{jk}(\nu_{jk} / (1)) - \varepsilon g_{jk}(0)(0) = (1) g_{jk}(\nu_{jk} / (1)) \leq 0$$

c. The LHS of the new constraints are **convex**.

Convex Relaxation Problem (CRP)

CRP:

$$\min Z = \sum_{k\in K}\sum_{j\in J_k}\gamma_{jk}\lambda_{jk} + f(x)$$

$$s.t. \qquad r(x) \le 0$$

$$x = \sum_{j\in J_k} \nu^{jk}, k \in K$$

$$0 \le \nu^{jk} \le \lambda_{jk} U_{jk}, j \in J_k, k \in K$$

$$\sum_{j\in J_k} \lambda_{jk} = 1 \ , k \in K$$

$$\lambda_{jk} g_{jk}(\nu^{jk}/\lambda_{jk}) \le 0, \quad j \in J_k, k \in K$$

Convex Hull Formulation

$$A\lambda \le a$$

Logic constraints

$$x, \nu^{jk} \ge 0, \ 0 \le \lambda_{jk} \le 1, \ j \in J_k, k \in K$$

- **Property**: ***The NLP (CRP) yields a lower bound to optimum of (GDP).***

Note: Hull relaxation as intersection of convex hull for each disjunction

Strength Lower Bounds

- **Theorem**: ***The relaxation of (CRP) yields a lower bound that is greater than or equal to the lower bound that is obtained from the relaxation of problem (BM):***

RBM:

$$\min Z = \sum_{k\in K}\sum_{j\in J_k} \gamma_{jk}\lambda_{jk} + f(x)$$

$$s.t. \quad r(x) \le 0$$

$$g_{jk}(x) \le M_{jk}(1-\lambda_{jk}) \quad j\in J_k, k\in K$$

$$\sum_{j\in J_k} \lambda_{jk} = 1, \; k\in K$$

$$A\lambda \le a$$

$$x \ge 0, \; 0 \le \lambda_{jk} \le 1$$

MINLP Reformulation

Specify in CRP λ as 0-1 variables

$$\min Z = \sum_{k\in K}\sum_{j\in J_k}\gamma_{jk}\lambda_{jk} + f(x)$$

$$s.t. \qquad r(x) \le 0$$

$$x = \sum_{j\in J_k} \nu^{jk}, k \in K$$

$$0 \le \nu^{jk} \le \lambda_{jk} U_{jk}, j \in J_k, k \in K$$

$$\sum_{j\in J_k} \lambda_{jk} = 1 \;, k \in K$$

$$\lambda_{jk} g_{jk}(\nu^{jk}/\lambda_{jk}) \le 0, \quad j \in J_k, k \in K$$

$$A\lambda \le a$$

$$x, \nu^{jk} \ge 0, \boxed{\lambda_{jk} = 0,1}\; j \in J_k, k \in K$$

Methods Generalized Disjunctive Programming

GDP

- **Logic based methods**
  - **Branch and bound**
    (Lee & Grossmann, 2000)
  - **Decomposition**
    Outer-Approximation
    Generalized Benders
    (Turkay & Grossmann, 1997)
- **Reformulation MINLP**
  Outer-Approximation
  Generalized Benders
  Extended Cutting Plane
  - **Convex-hull**
    Cutting plane
    (Sawaya & Grossmann, 2004)
  - **Big-M**

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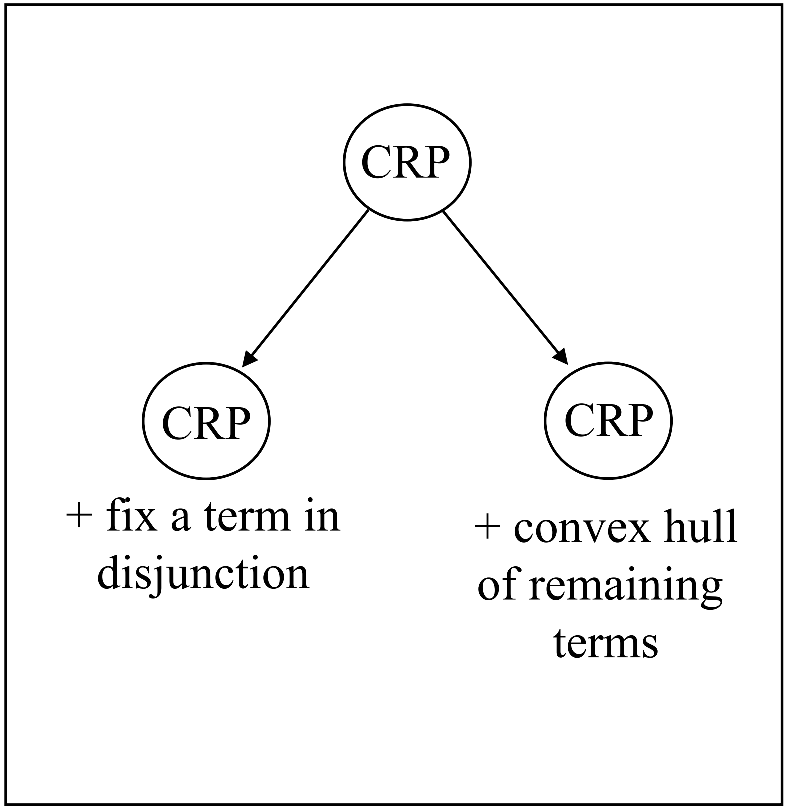
A Branch and Bound Algorithm for GDP

- **Tree Search**
  - **NLP subproblem at each node**
- **Solve CRP of GDP**
  - **lower bound**
- **Branching Rule**
  - **Set the largest λ_j as 1**
  - **Dichotomy rule**
- **Logic inference**

  ***CNF unit resolution** (Raman & Grosmann, 1993)*
- **Depth first search**

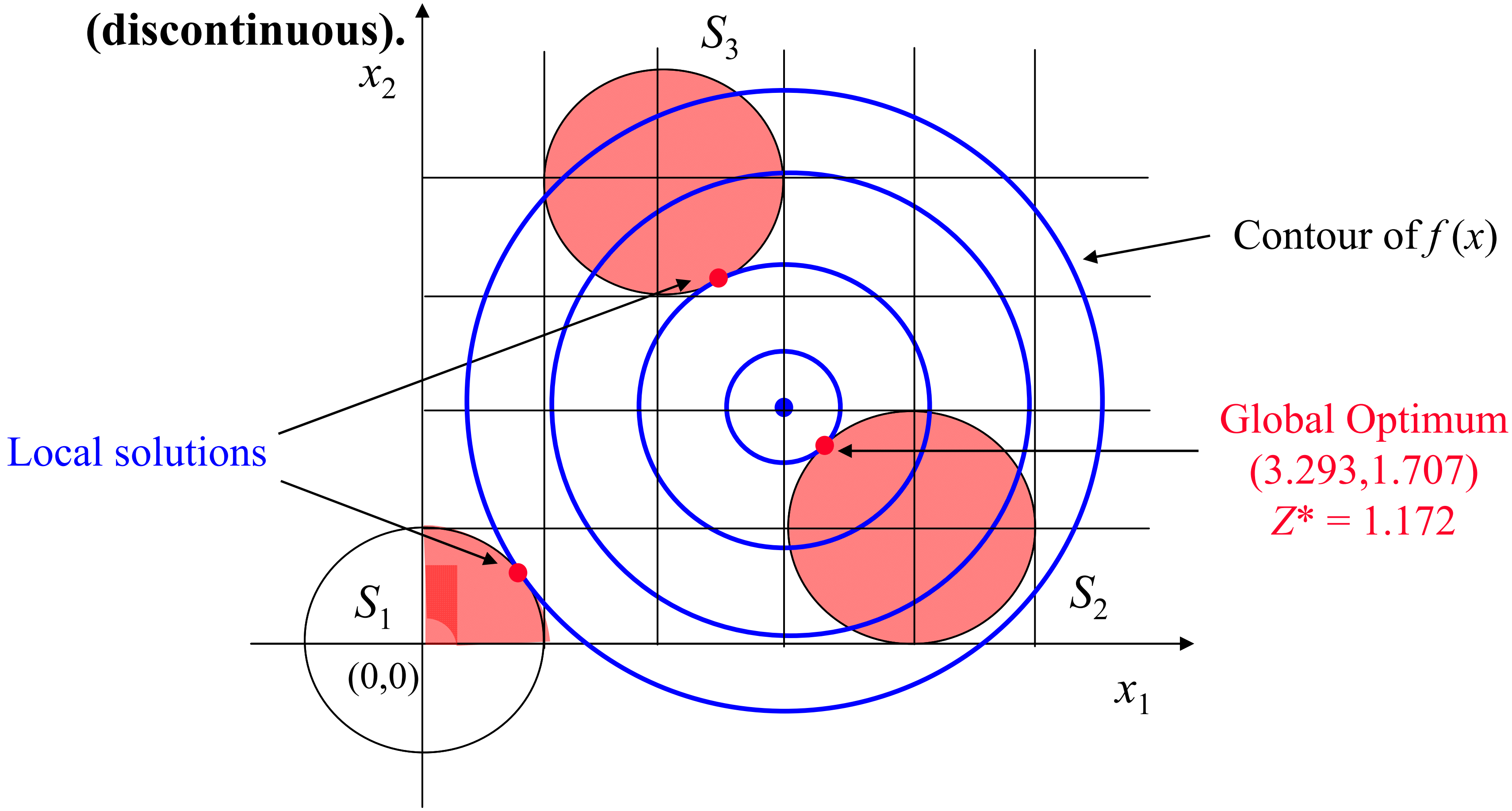
  When all the terms are fixed

  upper bound
- **Repeat Branching until $Z^L > Z^U$.**

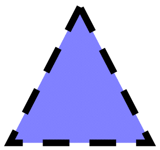


GDP Example

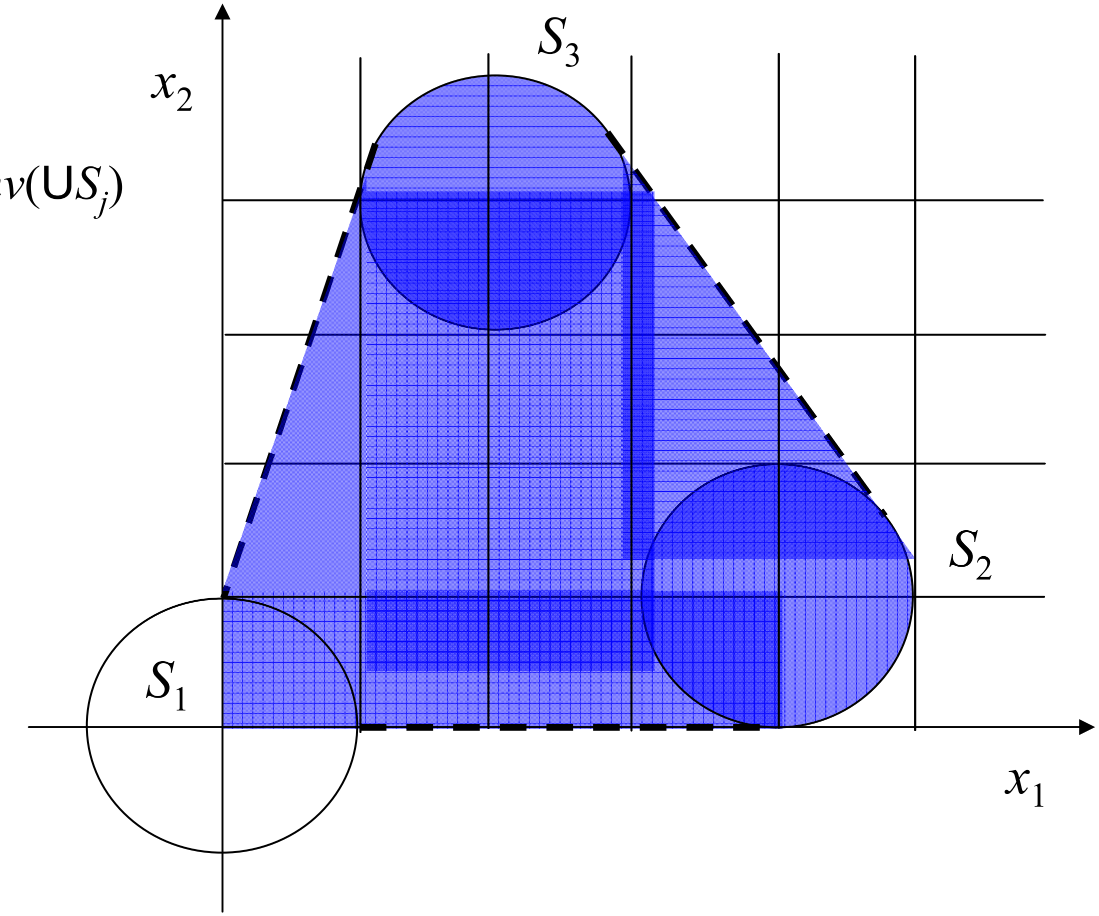
- Find $x \geq 0$, $(x \in S_1) \vee (x \in S_2) \vee (x \in S_3)$ to minimize $Z = (x_1 - 3)^2 + (x_2 - 2)^2 + c$
  - Objective Function = continuous function + fixed charge (discontinuous).



Example : convex hull



Convex hull = $conv(\cup S_j)$



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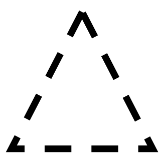
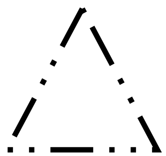
Example: CRP solution



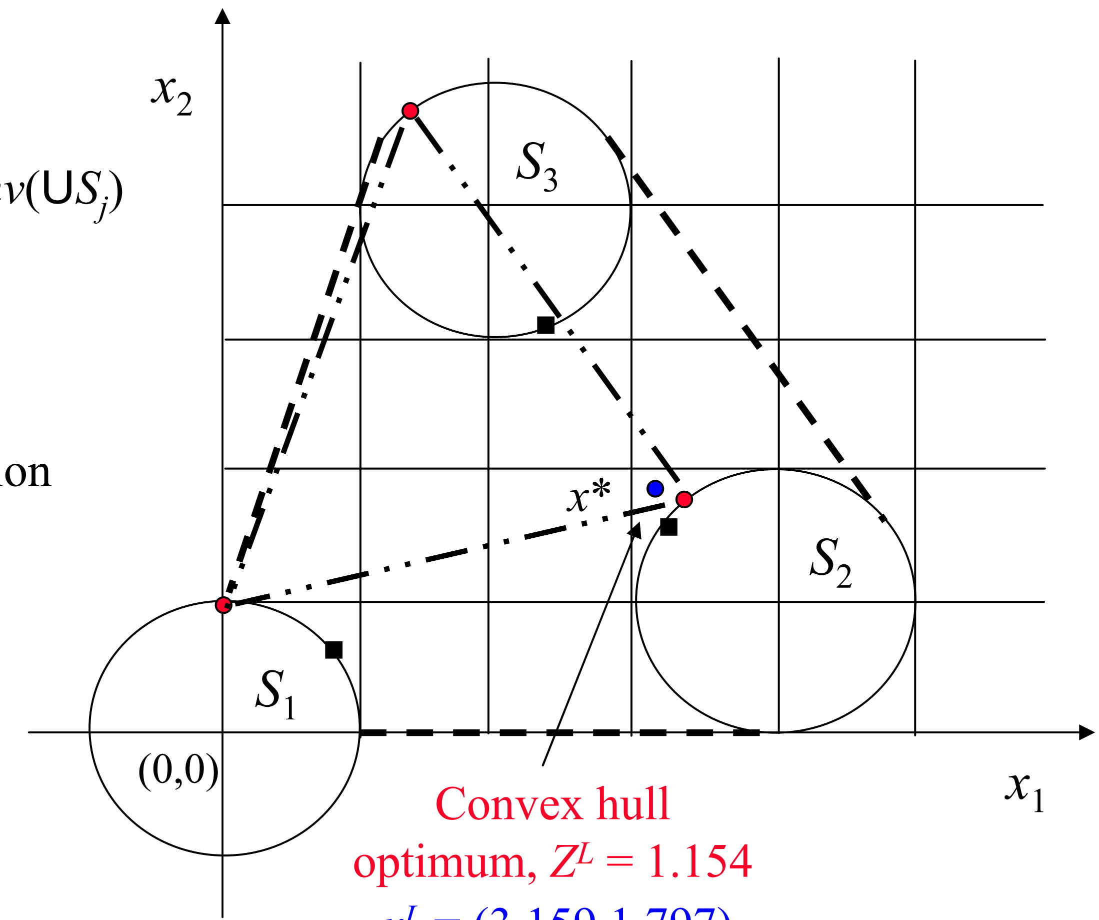
Convex hull = $conv(\cup S_j)$



Convex combination of z_j

$z_j = v^j/\lambda_j$

Local solution point



Convex hull optimum, $Z^L = 1.154$

$x^L = (3.159, 1.797)$

Infeasible to GDP

Weight

$\lambda_1 = 0.016$

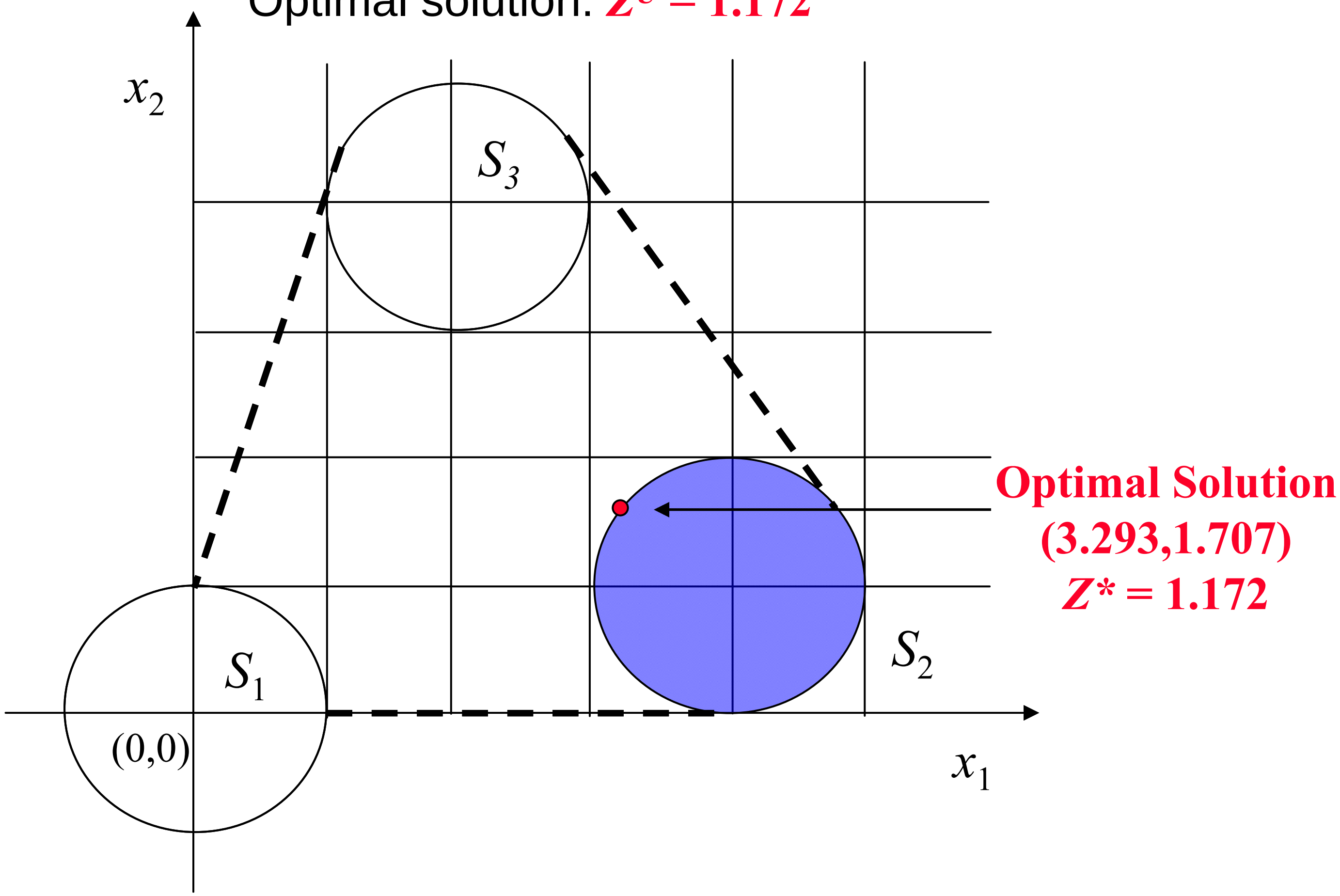
$\lambda_2 =$ **0.955**

$\lambda_3 = 0.029$

Example : branch and bound

First Node: S_2

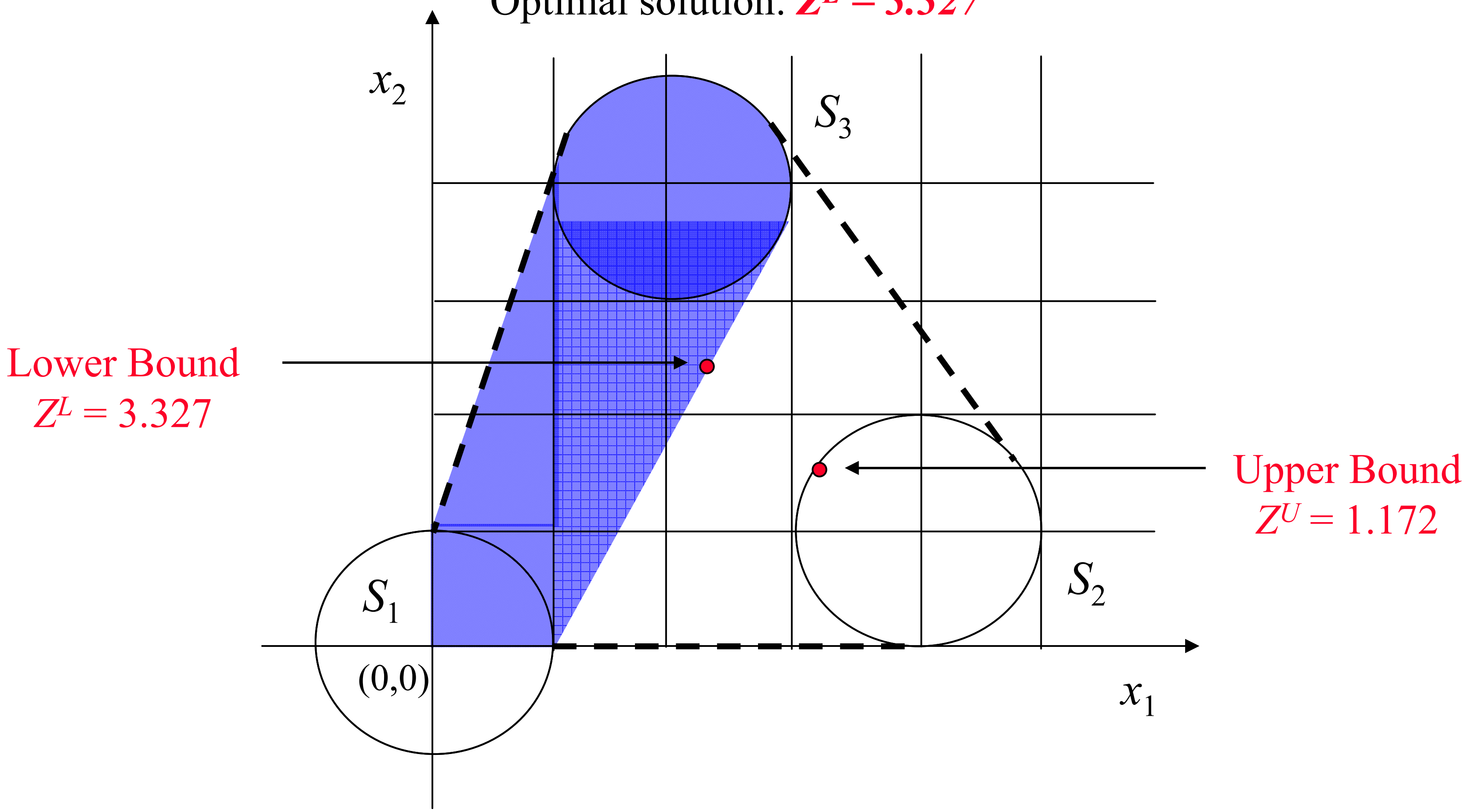
Optimal solution: $Z^U = 1.172$



Example : branch and bound

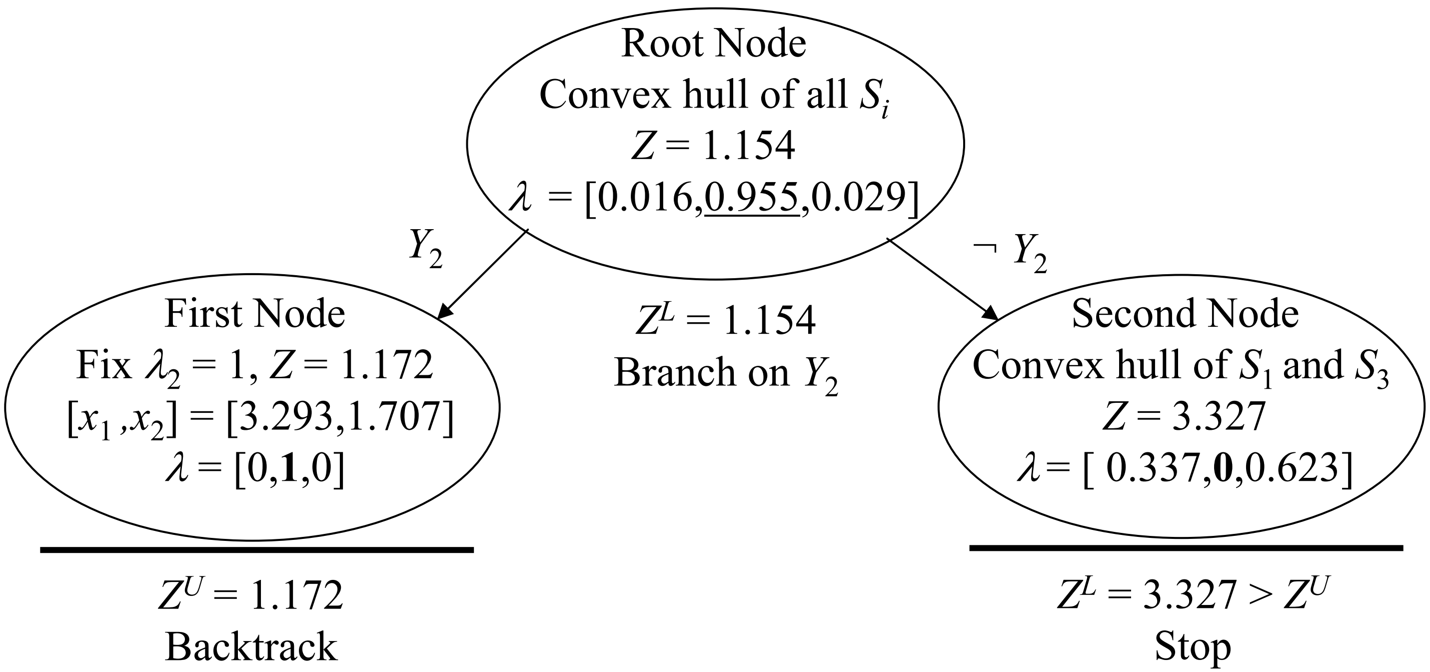
Second Node: ***conv(S_1 U S_3)***

Optimal solution: ***Z^L = 3.327***



Example: Search Tree

- **Branching Rule:** λ_j - the weight of disaggregated variable
  - Fix Y_j as true: fix λ_j as 1.



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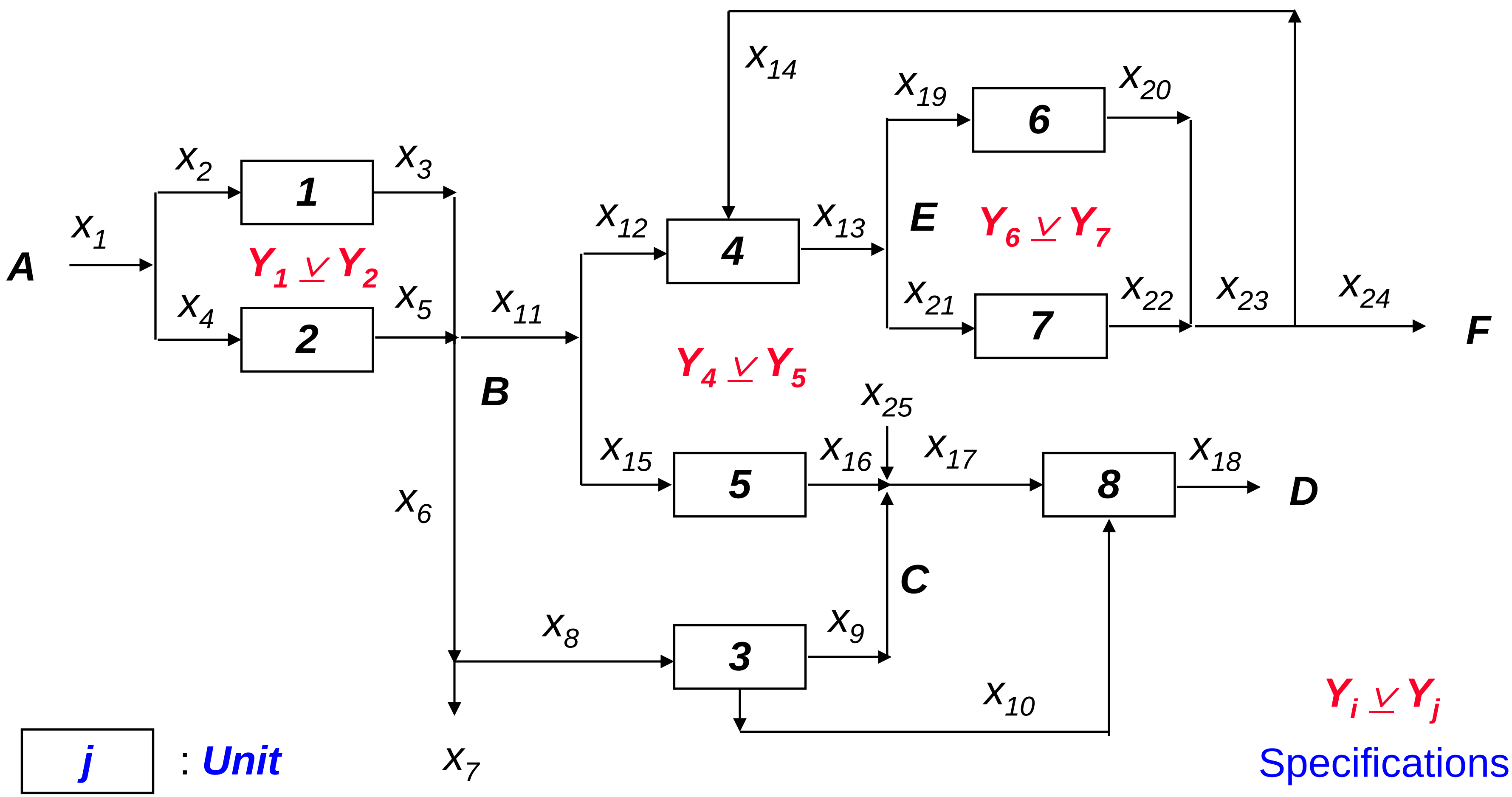
Process Network with Fixed Charges

- *Türkay and Grossmann (1997)*
  - **Superstructure of the process**



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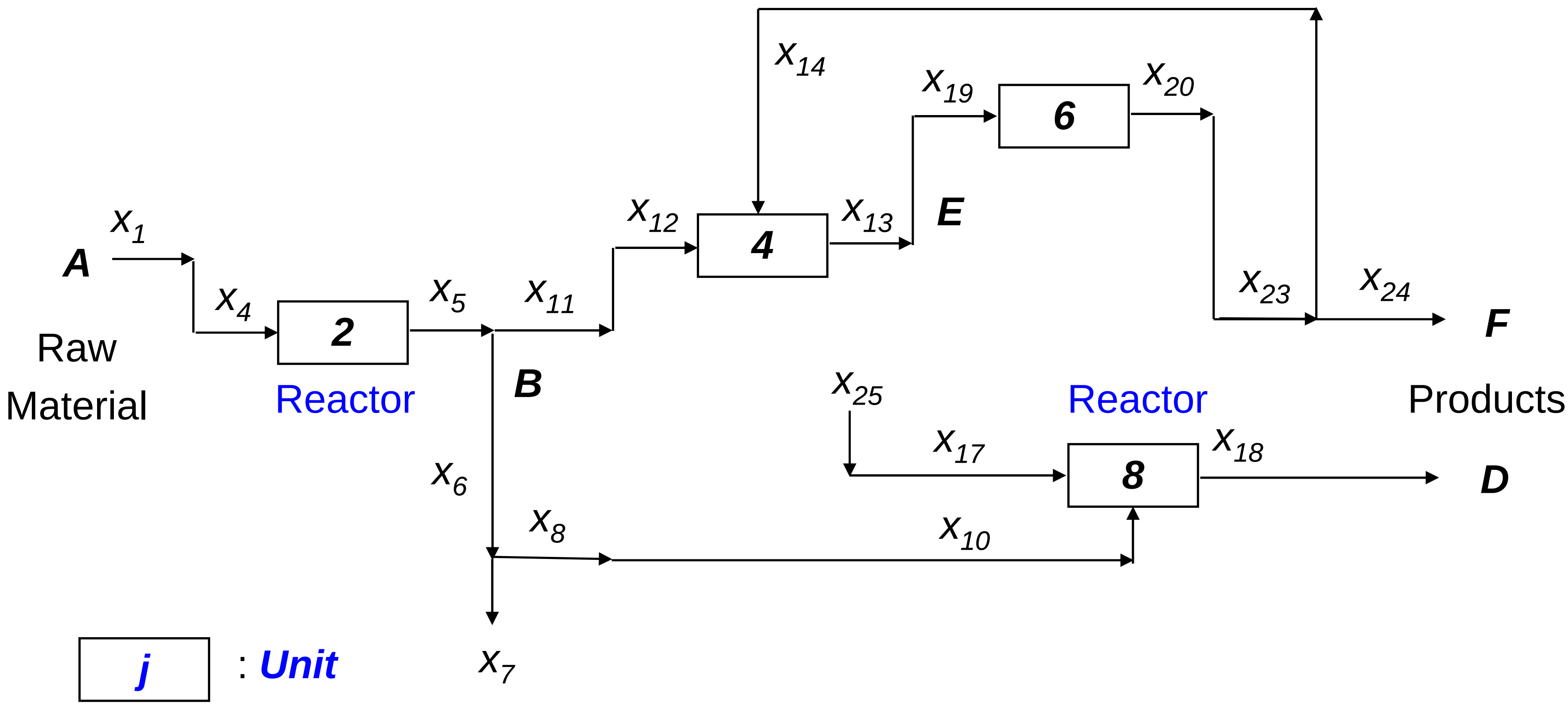
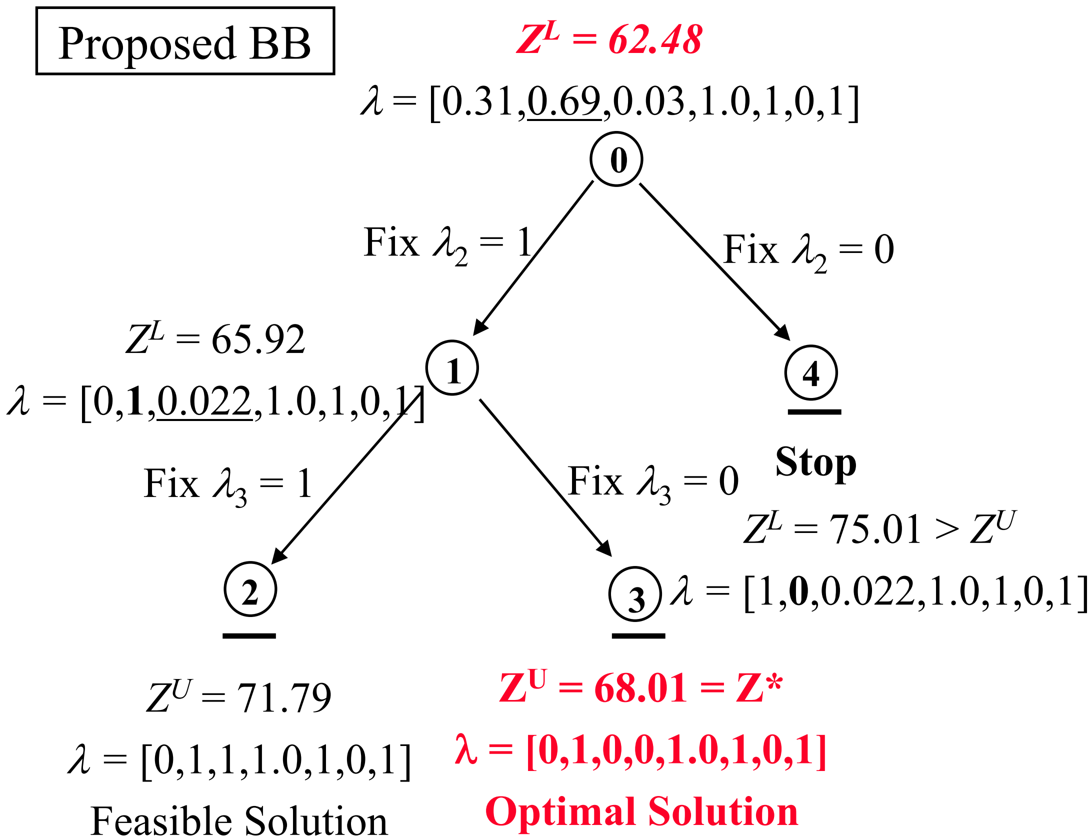
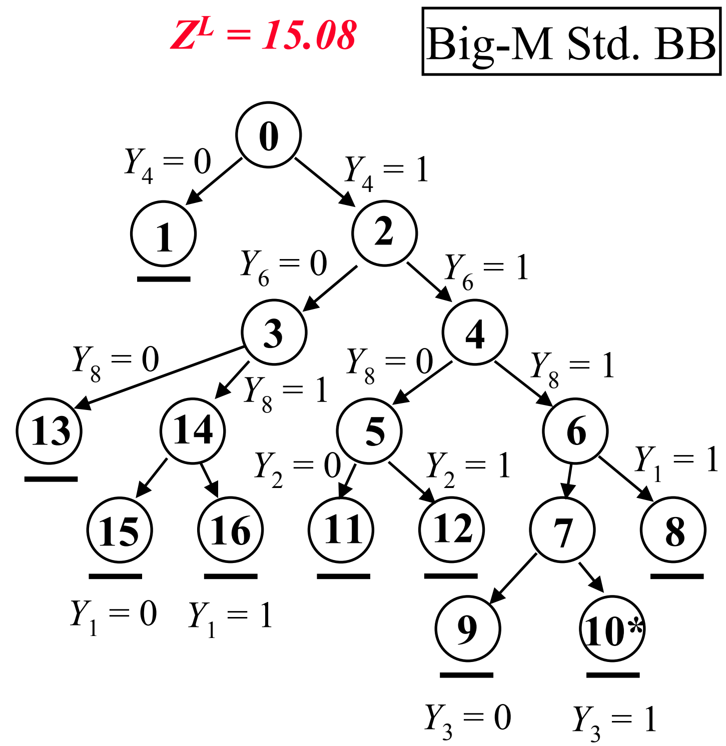
Optimal solution

- **Minimum Cost: $ 68.01M/year**



Proposed BB Method





- **5 nodes vs. 17 nodes of Standard BB (lower bound = 15.08)**

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Logic-based Outer Approximation

Main point: avoids solving MINLP in full space

Turkay, Grossmann (1997)

NLP Subproblem: (reduced)

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

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

$$\left.\begin{array}{l} h_{ik}(x) \le 0 \\ c_k = \gamma_{ik} \end{array}\right\} \text{for } Y_{\hat{i}k} = true \quad \hat{i} \in D_k, k \in SD \qquad \text{(NLPD)}$$

$$\left.\begin{array}{l} B^i x = 0 \\ c_k = 0 \end{array}\right\} \text{for } Y_{ik} = false \quad i \in D_k, i \ne \hat{i}, k \in SD$$

$$x \in R^n, \; c_i \in R^m,$$

Redundant constraints are eliminated with false values

Master Problem:

$$Min \quad Z = \sum_k c_k + \alpha$$

$$\text{s.t.}\quad \left.\begin{array}{l} \alpha \ge f(x^l) + \nabla f(x^l)^T (x - x^l) \\ g(x^l) + \nabla g(x^l)^T (x - x^l) \le 0 \end{array}\right\} \; l = 1,\dots,L \qquad \text{(MGDP)}$$

$$\bigvee_{i \in D_k} \left[\begin{array}{c} Y_{ik} \\ h_{ik}(x^l) + \nabla h_{ik}(x^l)^T (x - x^l) \le 0 \\ l \in L_{ik} \\ c_k = \gamma_{ik} \end{array}\right] \quad k \in SD$$

$$\Omega(Y) = True$$

$$\alpha \in R, \; x \in R^n, \; c \in R^m, \; Y \in \{true, false\}^m$$

Master problem solved with disjunctive branch and bound or with MILP reformulation

Proceed as OA. Requires initialization several NLPs to cover all disjunctions

LogMIP

Aldo Vecchietti, INGAR

Part of GAMS Modeling System

-Disjunctions specified with IF Then ELSE statements

```
DISJUNCTION D1(I,K,J);
D1(I,K,J)
      with (L(I,K,J)) IS
IF Y(I,K,J) THEN
      NOCLASH1(I,K,J);
ELSE
      NOCLASH2(I,K,J);
ENDIF;
```

-Logic can be specified in symbolic form (⇒, OR, AND, NOT)
or special operators (ATMOST, ATLEAST, EXACTLY)

-Linear case: MILP reformulation big-M, convex hull

-Nonlinear: Logic-based OA

http://www.ceride.gov.ar/logmip/

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Linear Generalized Disjunctive Programming
LGDP Model

Raman R. and Grossmann I.E. (1994) (Extension Balas (1979)) **(LGDP)**

$$\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x && \textit{Objective function}\\
&s.t. \qquad Bx \geq b && \textit{Common constraints}\\
&\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk} x \geq a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \qquad k \in K && \textit{Disjunctive constraints}\\
&\underline{\vee}_{j \in J_k} Y_{jk} \qquad k \in K &&\\
&\Omega(Y) = True && \textit{Logic constraints}\\
&x^L \leq x \leq x^U && \textit{Continuous variables}\\
&Y_{jk} \in \{True, False\} \qquad j \in J_k, k \in K && \textit{Boolean variables}\\
&c_k \in \mathbb{R}^1 \qquad k \in K &&
\end{aligned}$$

Logical OR operator

Can we obtain stronger relaxations?

Disjunctive Programming

Disjunction: A set of constraints connected to one another through the logical OR operator $\vee$

Conjunction: A set of constraints connected to one another through the logical AND operator $\wedge$

Constraint set of a DP can be expressed in two equivalent extreme forms

- **Disjunctive Normal Form (DNF)**
  - **A disjunction whose terms do not contain further disjunctions**

$$F = \left\{ x \in \mathbb{R}^n : \vee_{i \in Q} (A^i x \geq a^i) \right\}$$

- **Conjunctive Normal Form (CNF)**
  - **A conjunction whose terms do not contain further conjunctions**

$$F = \left\{ x \in \mathbb{R}^n : \widehat{A} x \geq \widehat{a}, \quad \vee_{h \in Q_j} (d^h x \geq d_0{}^h), \ j = 1, \ldots, t \right\}$$

Linear Generalized Disjunctive Programming
LGDP Model

(LGDP)

$$\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x && \textit{Objective function}\\
&s.t. \quad Bx \ge b && \textit{Common constraints}\\
&\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk} x \ge a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K && \textit{Disjunctive constraints}\\
&\underline{\vee}_{j \in J_k} Y_{jk} \quad k \in K && \textit{Logic constraints}\\
&\Omega(Y) = True &&\\
&x^L \le x \le x^U &&\\
&Y_{jk} \in \{True, False\} \quad j \in J_k, k \in K && \textit{Boolean variables}\\
&c_k \in \mathbb{R}^1 \quad k \in K &&
\end{aligned}$$

How to deal with Boolean and logic constraints in Disjunctive Programming?

Reformulating LGDP into Disjunctive Programming Formulation

Sawaya N.W. and Grossmann I.E. (2008)

$$
\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x \\
&s.t. \quad Bx \ge b \\
&\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk} x \ge a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \qquad k \in K \\
&\underset{j \in J_k}{\veebar} Y_{jk} \qquad k \in K \\
&\Omega(Y) = True \\
&x^L \le x \le x^U \\
&Y_{jk} \in \{True, False\} \qquad j \in J_k, k \in K \\
&c_k \in \mathbb{R}^1 \qquad k \in K
\end{aligned}
$$

LGDP

$$
\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x \\
&s.t. \quad Bx \ge b \\
&\bigvee_{j \in J_k} \begin{bmatrix} \lambda_{jk} = 1 \\ A^{jk} x \ge a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \qquad k \in K \\
&\sum_{j \in J_k} \lambda_{jk} = 1 \qquad k \in K \\
&H\lambda \ge h \\
&x^L \le x \le x^U \\
&0 \le \lambda_{jk} \le 1 \qquad j \in J_k, k \in K \\
&c_k \in \mathbb{R}^1 \qquad k \in K
\end{aligned}
$$

LDP ***=> Integrality λ guaranteed***

Proposition. LGDP and LDP have equivalent solutions.

Equivalent Forms in DP Through Basic Steps

There are many forms between CNF and DNF that are equivalent

Regular Form (RF): form represented by intersection of unions of polyhedra

Thus the RF is:

$$F = \bigcap_{t \in T} S_t$$

where for $t \in T, \quad S_t = \bigcup_{i \in Q_t} P_i, \quad P_i$ a polyhedron, $i \in Q_t$.

Proposition 1 (Theorem 2.1 in Balas (1979)). *Let F be a disjunctive set in RF. Then F can be brought to DNF by* $\underline{|T|-1}$ *<u>recursive applications of the following basic steps,</u> which preserve regularity:*

For some $r, s \in T, r \neq s,$ *bring* $S_r \cap S_s$ *to DNF, by replacing it with:*

$$S_{rs} = \bigcup_{\substack{i \in Q_r \\ t \in Q_s}} (P_i \cap P_t).$$

Illustrative Example: Basic Steps

$$F = S_1 \cap S_2 \cap S_3$$

$$S_1 = (P_{11} \cup P_{21}) \qquad S_2 = (P_{12} \cup P_{22}) \qquad S_3 = (P_{13} \cup P_{23})$$

Then F can be brought to DNF through 2 basic steps.

Apply Basic Step to:

$$S_1 \cap S_2 = (P_{11} \cup P_{21}) \cap (P_{12} \cup P_{22})$$

$$S_{12} = (P_{11} \cap P_{12}) \cup (P_{11} \cap P_{22}) \cup (P_{21} \cap P_{12}) \cup (P_{21} \cap P_{22})$$

We can then rewrite

$$F = S_1 \cap S_2 \cap S_3 \qquad \text{as } F = S_{12} \cap S_3$$

Apply Basic Step to:

$$S_{12} \cap S_3 = ((P_{11} \cap P_{12}) \cup (P_{11} \cap P_{22}) \cup (P_{21} \cap P_{12}) \cup (P_{21} \cap P_{22})) \cap (P_{13} \cup P_{23})$$

$$S_{123} = \begin{pmatrix} (P_{11} \cap P_{12} \cap P_{13}) \cup (P_{11} \cap P_{22} \cap P_{13}) \cup (P_{21} \cap P_{12} \cap P_{13}) \cup (P_{21} \cap P_{22} \cap P_{13}) \\ \cup (P_{11} \cap P_{12} \cap P_{23}) \cup (P_{11} \cap P_{22} \cap P_{23}) \cup (P_{21} \cap P_{12} \cap P_{23}) \cup (P_{21} \cap P_{22} \cap P_{23}) \end{pmatrix}$$

We can then rewrite

$$F = S_{12} \cap S_3 \qquad \text{as } F = S_{123}$$

which is its equivalent DNF

Equivalent Forms for GDP

$$
\begin{aligned}
&Min\ Z = \sum_{k\in K} c_k + d^T x \\
&s.t. \quad Bx \ge b \\
&\bigvee_{j\in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk}x \ge a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} && k \in K \\
&\underset{j\in J_k}{\underline{\vee}}\ Y_{jk} && k \in K \\
&\Omega(Y) = True \\
&x^L \le x \le x^U \\
&Y_{jk} \in \{True, False\} && j \in J_k, k \in K \\
&c_k \in \mathbb{R}^1 && k \in K
\end{aligned}
$$

LGDP

$\Rightarrow$

$$
\begin{aligned}
&Min\ Z = \sum_{k\in K} c_k + d^T x \\
&s.t. \quad Bx \ge b \\
&\bigvee_{j\in J_k} \begin{bmatrix} \lambda_{jk} = 1 \\ A^{jk}x \ge a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} && k \in K \\
&\sum_{j\in J_k} \lambda_{jk} = 1 && k \in K \\
&H\lambda \ge h \\
&x^L \le x \le x^U \\
&0 \le \lambda_{jk} \le 1 && j \in J_k, k \in K \\
&c_k \in \mathbb{R}^1 && k \in K
\end{aligned}
$$

LDP

$\Downarrow$

$$F = \left\{ z := (x,\lambda,c) \in \mathbb{R}^{n+\sum_{k\in K}|J_k|+|K|} : \bigcap_{i\in \bar{T}} \bar{b}^i z \ge \bar{b}_0^i \bigcap_{k\in K} \bigcup_{j\in J_k} (\bar{A}^{jk} z \ge \bar{a}^{jk}) \right\}$$

$\Downarrow$

All possible equivalent forms for GDP, obtained through any number of basic steps, are represented by:

LDP'

$$F = \left\{ z := (x,\lambda,c) \in \mathbb{R}^{n+\sum_{k\in K}|J_k|+|K|} : \bigcap_{i\in \hat{T}} \bar{b}^i z \ge \bar{b}_0^i \bigcap_{k\in \tilde{K}} \bigcup_{j\in J_k} (\tilde{A}^{jk} z \ge \tilde{a}^{jk}) \bigcap_{n\in \hat{K}} \bigcup_{m\in J_n} (\hat{A}^{mn} z \ge \hat{a}^{mn}) \right\}$$

Converting LDP to MIP reformulations

Proposition 2 (Theorem 3.3 combined with Corollary 3.5 in Balas (1979)). Let $F = \bigcup_{i \in Q} P_i,\ \ P_i = \left\{ x \in \mathbb{R}^n : \tilde{A}^i x \geq \tilde{a}_0{}^i \right\},\ i \in Q$, where Q is an arbitrary set and each $(\tilde{A}^i, \tilde{a}_0{}^i)$ is an $m_i \times (n+1)$ matrix such that every P_i is a *bounded non-empty* polyhedron.

Furthermore, let $\zeta(Q)$ be the set of all those $x \in \mathbb{R}^n$ such that there exist vectors $(v^i, y_i) \in \mathbb{R}^{n+1}$, $i \in Q$, satisfying

$$x - \sum_{i \in Q} v^i = 0 \longrightarrow v^i$$

disaggregated variables

$$\begin{aligned} &\tilde{A}^i v^i - \tilde{a}_0{}^i y_i \geq 0 && i \in Q \\ &y_i \geq 0 && i \in Q \\ &\sum_{i \in Q} y_i = 1 && i \in Q \end{aligned}$$

=> Convex Hull

Then $cl\ conv\ F = \zeta(Q)$.

Proposition 3 (Corollary 3.7 in Balas (1979).

Let $\zeta_I(Q) := \left\{ x \in \zeta(Q) : y_i \in \{0,1\},\ i \in Q \right\}$.

=> MIP representation

Then $\zeta_I(Q) = F$.

Family of MIP Reformulations For GDP

$$F=\left\{z:=(x,\lambda,c)\in\mathbb{R}^{n+\sum_{k\in K}|J_k|+|K|}:\bigcap_{i\in\bar{T}}\bar{b}^i z\ge\bar{b}_0^i\bigcap_{k\in\tilde{K}}\bigcup_{j\in J_k}(\tilde{A}^{jk}z\ge\tilde{a}^{jk})\bigcap_{n\in\hat{K}}\bigcup_{m\in J_n}(\hat{A}^{mn}z\ge\hat{a}^{mn})\right\}$$

LDP'

General template for any MILP reformulation

$$Min\ Z=\sum_{k\in K}\sum_{j\in J_k}\gamma_{jk}y_{jk}+d^T x$$

$s.t.$

$$b^i x\ge b_0^i \qquad i\in I_{B_1}$$
$$h^i y\ge h_0^i \qquad i\in I_{H_1}$$
$$x_i^L\le x_i\le x_i^U \qquad i\in I_{X_1}$$
$$y_{jk}=\sum_{m\in J_n}\hat{u}_{jk}^{mn} \qquad (j,k)\in L_{2_n}\cup K_{S_{2_n}}\cup I_{H_{2_n}},n\in N$$
$$x=\sum_{m\in J_n}\hat{v}^{mn} \qquad n\in N$$
$$b^i\hat{v}^{mn}\ge b_0^i\hat{y}_{mn} \qquad i\in I_{B_{2_n}},m\in J_n,n\in N$$
$$\sum_{j\in J_k}\hat{u}_{jk}^{mn}=\hat{y}_{mn} \qquad k\in K_{S_{2_n}},m\in J_n,n\in N$$
$$h^i\hat{u}^{mn}\ge h_0^i\hat{y}_{mn} \qquad i\in I_{H_{2_n}},m\in J_n,n\in N$$
$$\hat{u}_{jk}^{mn}=\hat{y}_{mn} \qquad (j,k)\in M_{mn},m\in J_n,n\in N$$
$$A^{jk}\hat{v}^{mn}\ge a^{jk}\hat{y}_{mn} \qquad (j,k)\in M_{mn},m\in J_n,n\in N$$
$$x^L\hat{y}_{mn}\le\hat{v}^{mn}\le x^U\hat{y}_{mn} \qquad m\in J_n,n\in N$$
$$0\le\hat{u}_{jk}^{mn}\le\hat{y}_{mn} \qquad (j,k)\in L_{3_n},m\in J_n,n\in N$$
$$\sum_{m\in J_n}\hat{y}_{mn}=1 \qquad n\in N$$
$$\sum_{m\in Q_{n_{jk}}}\hat{y}_{mn_{jk}}=y_{jk} \qquad n_{jk}\in N,j\in J_k,k\in K$$
$$\sum_{j\in J_k}y_{jk}=1 \qquad k\in K$$
$$\hat{y}_{mn}\ge 0 \qquad m\in J_n,n\in N$$
$$y_{jk}\in\{0,1\} \qquad j\in J_k,k\in K$$

MIP'

Particular case: Convex Hull Reformulation of LGDP

Raman and Grossmann I.E. (1994)

(CH)

$$Min\ Z = \sum_{k \in K} \sum_{j \in J_k} \gamma_{jk} y_{jk} + d^T x$$

Disaggregated variables

$$
\begin{array}{ll}
s.t. \quad Bx \geq b & \\
x = \sum_{j \in J_k} v^{jk} & k \in K \\
A^{jk} v^{jk} \geq a^{jk} y_{jk} & j \in J_k, k \in K \\
x^L y_{jk} \leq v^{jk} \leq x^U y_{jk} & j \in J_k, k \in K \\
\sum_{j \in J_k} y_{jk} = 1 & k \in K \\
Hy \geq h & \\
y_{jk} \in \{0,1\} & j \in J_k, k \in K
\end{array}
$$

While this MILP formulation has stronger relaxation than big-M, it is not strongest!!

A Hierarchy of Relaxations for GDP

Proposition 4. *For* $i \in \bar{T}| + |K| - 1$ *let* F_{GDP_i} *be a sequence of regular forms of the disjunctive set:*

$$F = \left\{ z := (x,\lambda,c) \in \mathbb{R}^{n+\sum_{k\in K}|J_k|+|K|} : \bigcap_{i\in\bar{T}} \bar{b}^i z \ge \bar{b}_0^i \bigcap_{k\in\tilde{K}} \bigcup_{j\in J_k} (\tilde{A}^{jk} z \ge \tilde{a}^{jk}) \bigcap_{n\in\hat{K}} \bigcup_{m\in J_n} (\hat{A}^{mn} z \ge \hat{a}^{mn}) \right\},\ \textit{such that}$$

i) F_{GDP_0} *corresponds to the disjunctive form:*

$$F = \left\{ z := (x,\lambda,c) \in \mathbb{R}^{n+\sum_{k\in K}|J_k|+|K|} : \bigcap_{i\in\bar{T}} \bar{b}^i z \ge \bar{b}_0^i \bigcap_{k\in K} \bigcup_{j\in J_k} (\bar{A}^{jk} z \ge \bar{a}^{jk}) \right\};$$

ii) $F_{GDP_{|\bar{T}|+|K|-1}} := F_t$ *is in DNF;*

iii) for $i = 1,\ldots,t,$ F_{GDP_i} *is obtained from* $F_{GDP_{i-1}}$ *by a basic step.*

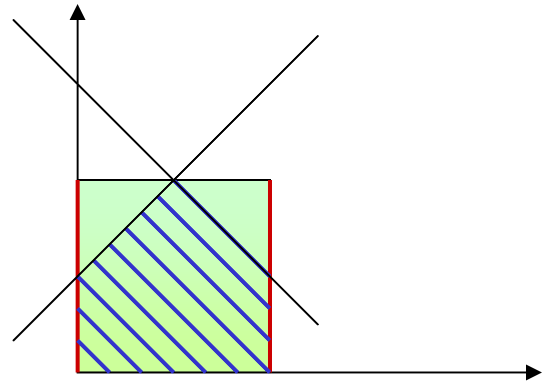
Then,

$h-rel\ F_{GDP_0} \supseteq h-rel\ F_{GDP_1} \supseteq \cdots \supseteq h-rel\ F_{GDP_{|\bar{T}|+|K|-1}} = clconv\ F_{GDP_{|\bar{T}|+|K|-1}} = clconv\ F_t$. ***(true convex hull)***

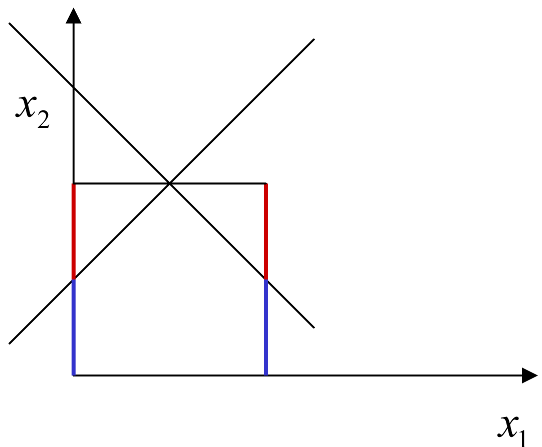
Illustrative Example:
Hierarchy of Relaxations

$$x_1 - x_2 + 0.5 \geq 0$$
$$-x_1 - x_2 + 1 \geq 0$$
$$\begin{bmatrix} x_1 = 0 \\ 0 \leq x_2 \leq 1 \end{bmatrix} \vee \begin{bmatrix} x_1 = 1 \\ 0 \leq x_2 \leq 1 \end{bmatrix}$$

Convex Hull of disjunction



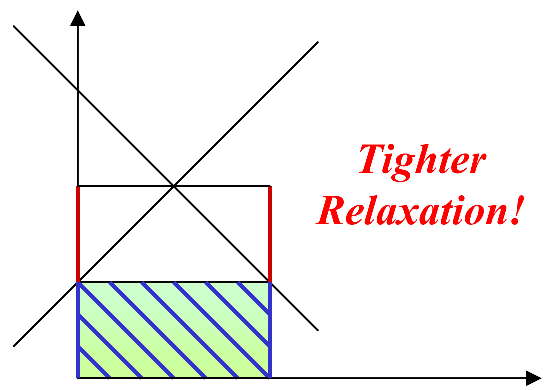
LP Relaxation



Application of 2 Basic Steps

$$\begin{bmatrix} x_1 - x_2 + 0.5 \geq 0 \\ -x_1 - x_2 + 1 \geq 0 \\ x_1 = 0 \\ 0 \leq x_2 \leq 1 \end{bmatrix} \vee \begin{bmatrix} x_1 - x_2 + 0.5 \geq 0 \\ -x_1 - x_2 + 1 \geq 0 \\ x_1 = 1 \\ 0 \leq x_2 \leq 1 \end{bmatrix}$$

Convex Hull of disjunction



Tighter Relaxation!

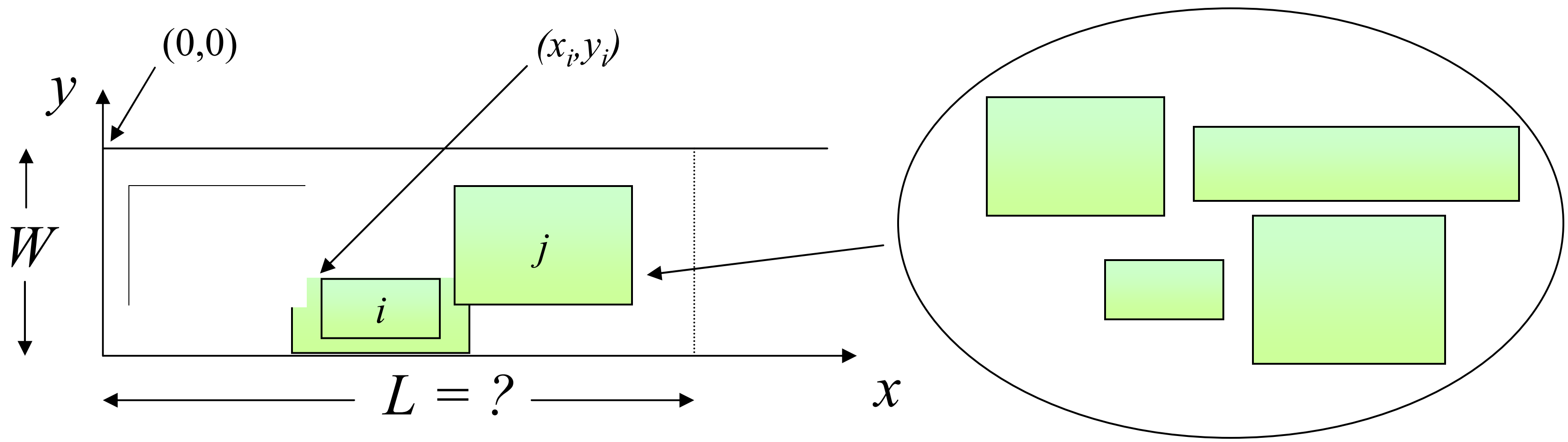
Numerical Example: Strip-packing problem

Problem statement: *Hifi (1998)*

Given a set of small rectangles with width H_i and length L_i.

Large rectangular strip of fixed width W and unknown length L.

Objective is to fit small rectangles onto strip without overlap and rotation while **minimizing length L of the strip.**



Set of small rectangles

GDP/DP Model for Strip-packing problem

$$
\begin{aligned}
&Min \quad lt \\
&s.t. \quad lt \geq x_i + L_i && \forall i \in N \\
&\begin{bmatrix} Y^1_{ij} \\ x_i + L_i \leq x_j \end{bmatrix} \vee \begin{bmatrix} Y^2_{ij} \\ x_j + L_j \leq x_i \end{bmatrix} \vee \begin{bmatrix} Y^3_{ij} \\ y_i - H_i \geq y_j \end{bmatrix} \vee \begin{bmatrix} Y^4_{ij} \\ y_j - H_j \geq y_i \end{bmatrix} && \forall i,j \in N, i<j \\
&x_i \leq UB_i - L_i && \forall i \in N \\
&H_i \leq y_i \leq W && \forall i \in N \\
&lt, x_i, y_i \in \mathbb{R}^1_+ ,\ Y^1_{ij}, Y^2_{ij}, Y^3_{ij}, Y^4_{ij} \in \{True, False\} && \forall i,j \in N, i<j
\end{aligned}
$$

Objective function
Minimize length

Disjunctive constraints
No overlap between rectangles

Bounds on variables

$\Downarrow$

$$
\begin{aligned}
&Min \quad lt \\
&s.t. \quad lt \geq x_i + L_i && \forall i \in N \\
&\begin{bmatrix} \lambda^1_{ij} = 1 \\ x_i + L_i \leq x_j \end{bmatrix} \vee \begin{bmatrix} \lambda^2_{ij} = 1 \\ x_j + L_j \leq x_i \end{bmatrix} \vee \begin{bmatrix} \lambda^3_{ij} = 1 \\ y_i - H_i \geq y_j \end{bmatrix} \vee \begin{bmatrix} \lambda^4_{ij} = 1 \\ y_j - H_j \geq y_i \end{bmatrix} && \forall i,j \in N, i<j \\
&\lambda^1_{ij} + \lambda^2_{ij} + \lambda^3_{ij} + \lambda^4_{ij} = 1 \quad \forall i,j \in N, i<j \\
&x_i \leq UB_i - L_i && \forall i \in N \\
&H_i \leq y_i \leq W && \forall i \in N \\
&lt, x_i, y_i \in \mathbb{R}^1_+ ,\ 0 \leq \lambda^1_{ij}, \lambda^2_{ij}, \lambda^3_{ij}, \lambda^4_{ij} \leq 1 && \forall i,j \in N, i<j
\end{aligned}
$$

25 Rectangle Problem Optimal solution= 31

Original CH		Strengthened
1,112 0-1 variables	=>	1,112 0-1 variables
4,940 cont vars		5,783 cont vars
7,526 constraints		8,232 constraints
LP relaxation = 9		LP relaxation = 27!

31 Rectangle Problem Optimal solution= 38

Original CH		Strengthened
2,256 0-1 variables	=>	2,256 0-1 variables
9,716 cont vars		11,452 cont vars
14,911 constraints		15,624 constraints
LP relaxation = 10.64		LP relaxation = 33!

Cutting Planes for Linear Generalized Disjunctive Programming

GDP Model:

Sawaya, Grossmann (2004)

$$Min\ Z = \sum_{k \in K} c_k + h^T x$$

Objective Function

$$s.t. \quad Bx \le b$$

Common Constraints

OR Operator

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A_{jk} x \le a_{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$

Disjunctive Constraints

$$\Omega(Y) = True$$

Logic Constraints

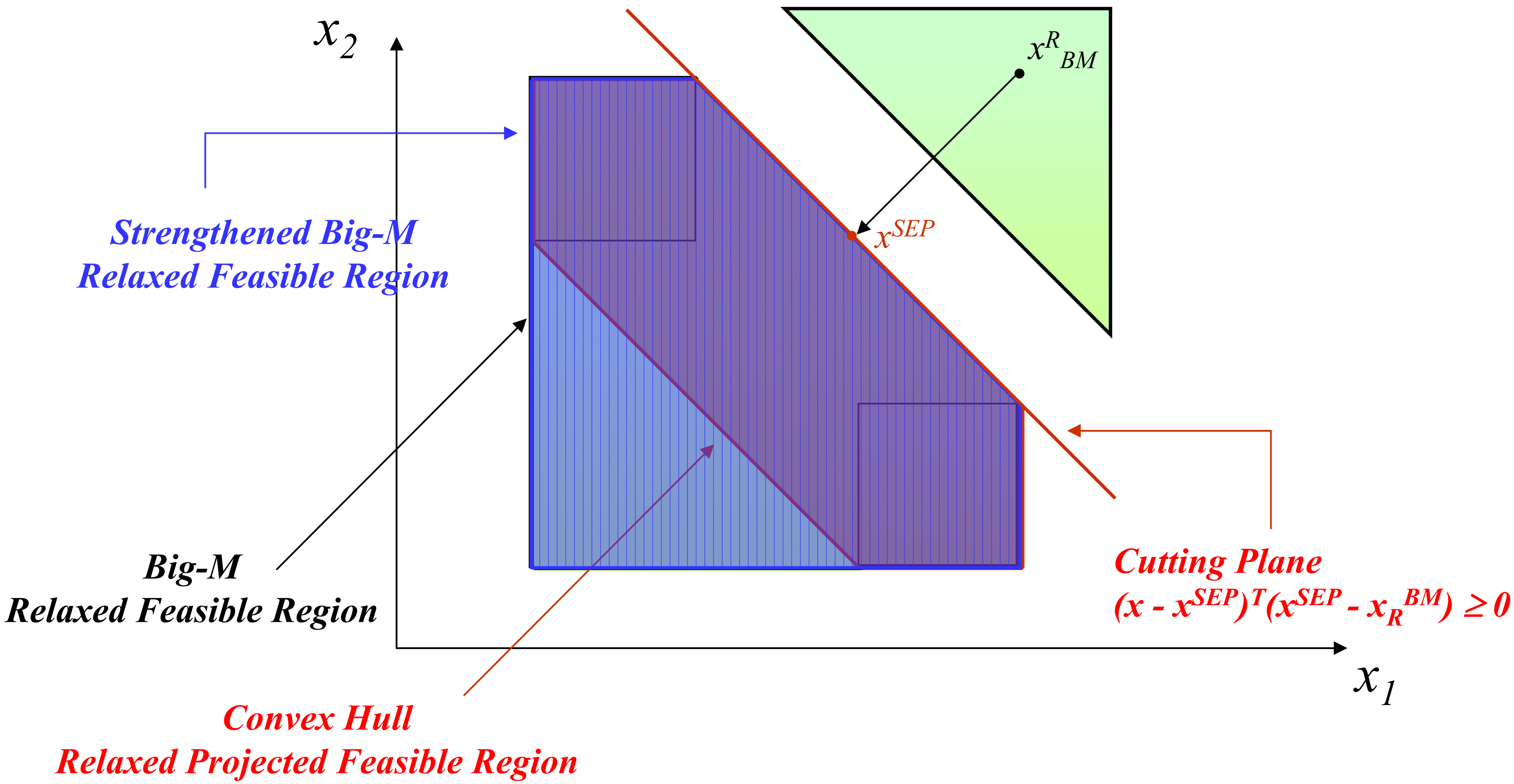
$$x \in R^n,\ Y_{jk} \in \{True, False\},\ c_k \in R$$

$$j \in J_k,\ k \in K$$

Boolean Variables

Motivation for Cutting Plane Method

Trade-off: ***Big-M fewer vars/weaker relaxation vs Convex-Hull tighter relaxation/more vars***



Global Optimization Algorithms

- **Most algorithms are based on spatial branch and bound method** **(Horst & Tuy, 1996)**

- **Nonconvex NLP/MINLP**
  - **αBB** **(Adjiman, Androulakis & Floudas, 1997; 2000)**
  - **BARON (Branch and Reduce)** **(Ryoo & Sahinidis, 1995, Tawarmalani and Sahinidis (2002))**
  - **OA for nonconvex MINLP** **(Kesavan et al., 2004)**
  - **Branch and Contract** **(Zamora & Grossmann, 1999)**

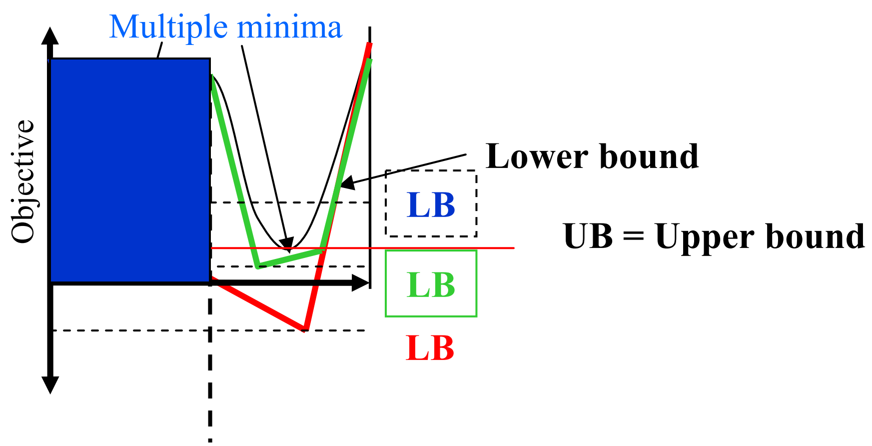
- **Nonconvex GDP**
  - **Two-level Branch and Bound** **(Lee & Grossmann, 2001)**

Spatial Branch and Bound to

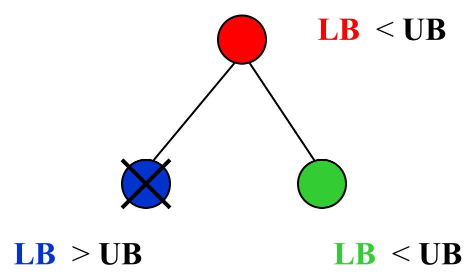
obtain the Global Optimum

- Guaranteed to converge to global optimum given a certain tolerance between lower and upper bounds

Global optimum search



Branch and bound tree



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Nonconvex GDP

$$\min \quad Z = \sum_k c_k + f(x)$$
Objective Function

$$s.t. \quad r(x) \le 0$$
Common Constraints

OR operator →
$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix}, k \in K$$
Disjunctions

$$\Omega(Y) = true$$
Logic Propositions

$$x \in R^n, c_k \in R^1$$

$$Y_{jk} \in \{true, \ false\}$$

f, g and r: nonconvex

Convex Underestimator GDP (R)

- Introducing convex underestimators

$$\min \; Z = \sum_k c_k + \overline{f}(x)$$

$$s.t. \quad \overline{r}(x) \le 0$$

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ \overline{g}_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix}, k \in K$$

$$\Omega(Y) = true$$

$$x \in R^n, c_k \in R^1$$

$$Y_{jk} \in \{true, \; false\}$$

$$\overline{f}, \overline{r} \; and \; \overline{g} : convex$$

Convex underestimators

Bilinear: Linear

McCormick (1976), Al-Khayyal (1992)

Linear fractional: Convex nonlinear

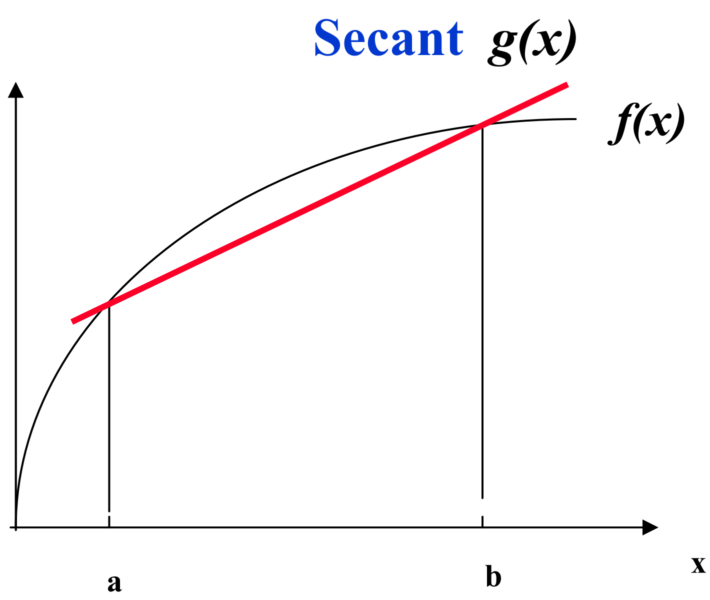
Quesada and Grossmann (1995)

Concave separable: Linear secant

- Problem (R) yields a valid lower bound to Problem (GDP)

Convex envelopes

Concave function



$$g(x) = f(a) + \frac{[f(b) - f(a)]}{b - a}(x - a)$$

Bilinear

$$w = xy$$

$$x^L \le x \le x^U \qquad y^L \le y \le y^U$$

McCormick convex envelopes

$$w \ge x^L y + y^L x - x^L y^L$$
$$w \ge x^U y + y^U x - x^U y^U$$
$$w \le x^L y + y^U x - x^L y^U$$
$$w \le x^U y + y^L x - x^U y^L$$

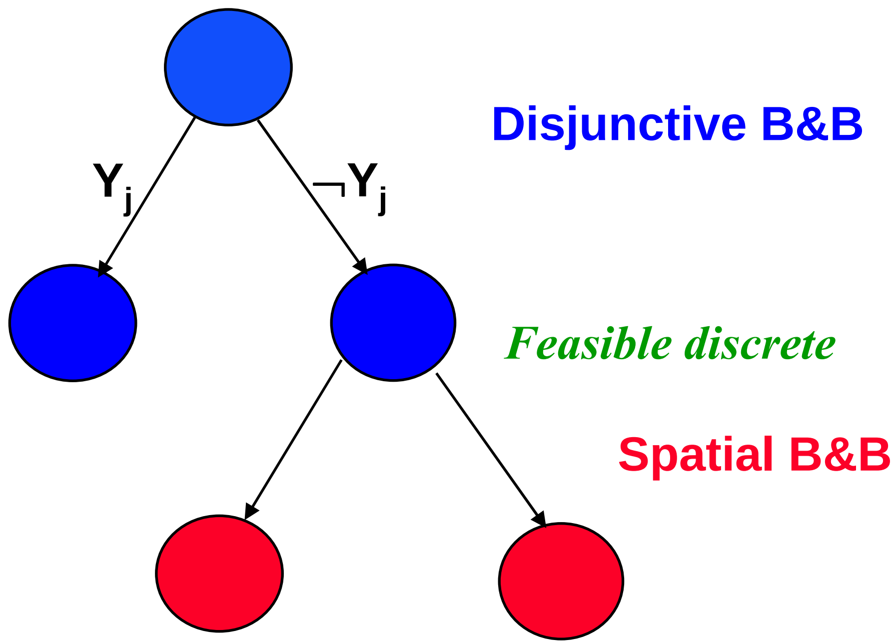
For other convex envelopes/underestimators see:

Tawarmalani, M. and N. V. Sahinidis, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications*, Vol. 65, *Nonconvex Optimization And Its Applications* series, Kluwer Academic Publishers, Dordrecht, 2002

Basic Ideas Global Optimization GDP

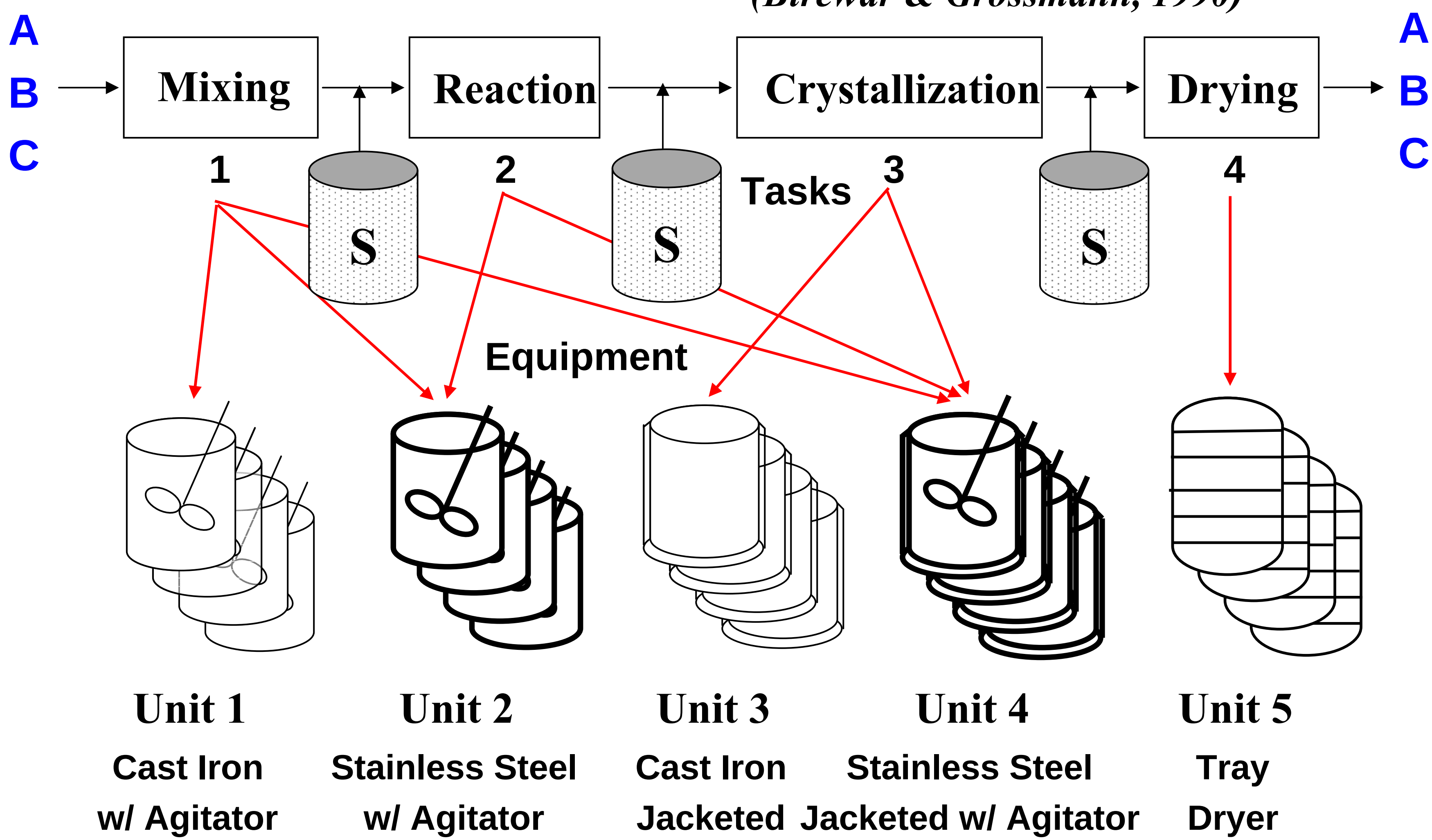
1. **Branch and bound enumeration on disjunctions of convex GDP (*R*)**

2. **When feasible discrete solution found switch to spatial branch and bound (NLP subproblem)**



Synthesis Multiproduct Batch Plant

(Birewar & Grossmann, 1990)



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More than 100 alternatives: each requires nonlinear optimization

Synthesis Multiproduct Batch Plant

Nonconvex GDP Model

$$\min \boxed{\mathrm{COST} = \sum_{j=1}^{M} N_j^{EQ} C_j + \sum_j CS_j}$$ **Objective function**

$$s.t. \quad V_t^T \geq B_i S_{it} \quad i = 1,\ldots,N_P; t = 1,\ldots,T$$ **Sizing**

$$pt_{ij} = \sum_{t \in T_j} pty_{itj} \quad i = 1,\ldots,N_P; j = 1,\ldots,M$$ **Process time**

$$n_i B_i \geq Q_i \quad i = 1,\ldots,N_P$$ **Demand**

$$\boxed{\sum_{i=1}^{N_P} n_i T_{Li} \leq H}$$ **Horizon time**

$$\bigvee_{j \in J_t} \begin{bmatrix} Y_{tj} \\ V_j \geq V_t^T \\ pty_{itj} = pt_{it}^T \\ pty_{itj'} = 0, j' \neq j \end{bmatrix} \quad t \in T$$

Disjunction for Task Assignments

$\boxed{}$ **Nonconvex functions**

GDP model (continued)

$$\begin{bmatrix} & & YEX_j & \\ & & \boxed{C_j = \gamma_j + \alpha_j V_j^{0.6}} & \\ & & V_j^L \le V_j \le V_j^U & \\ \begin{bmatrix} YC_{1j} \\ N_j^{EQ} = 1 \\ T_{Li} \ge pt_{ij} \end{bmatrix} \vee & \begin{bmatrix} YC_{2j} \\ N_j^{EQ} = 2 \\ 2T_{Li} \ge pt_{ij} \end{bmatrix} \vee & \begin{bmatrix} YC_{3j} \\ N_j^{EQ} = 3 \\ 3T_{Li} \ge pt_{ij} \end{bmatrix} \vee & \begin{bmatrix} YC_{4j} \\ N_j^{EQ} = 4 \\ 4T_{Li} \ge pt_{ij} \end{bmatrix} \end{bmatrix} \vee \begin{bmatrix} \neg YEX_j \\ C_j = 0 \\ V_j = 0 \\ N_j^{EQ} = 0 \\ pt_{ij} = 0 \\ T_{Li} \ge 0 \end{bmatrix} \quad j \in J$$

Disjunction for Equipment

$$\begin{bmatrix} YS_j \\ -\phi \le B_{ij} - B_{ij'} \le \phi \\ VST_j \ge S'_{ij} B_{ij} NEQ_j \\ VST_j \ge S'_{ij} B_{ij'} NEQ_{j'} \\ 100 \le VST_j \le 10000 \\ \boxed{CS_j = 5000 + 80 VST_j^{0.5}} \end{bmatrix} \vee \begin{bmatrix} \neg YS_j \\ B_{ij} = B_{ij'} \\ VST_j = 0 \\ CS_j = 0 \end{bmatrix} \quad j \in J$$

Disjunction for Storage Tank

$$YEX_1 \Leftrightarrow Y_{11}, YEX_2 \Leftrightarrow Y_{12} \vee Y_{22}, YEX_3 \Leftrightarrow Y_{33}$$

$$YEX_4 \Leftrightarrow Y_{14} \vee Y_{24} \vee Y_{34}, YEX_5 \Leftrightarrow Y_{45}$$

$$W_{04} \underline{\vee} W_{14} \underline{\vee} W_{24} \underline{\vee} W_{34}$$

$$W_{04} \Leftrightarrow \neg Y_{14} \wedge \neg Y_{24} \wedge \neg Y_{34}$$

$$W_{14} \Leftrightarrow (Y_{14} \wedge \neg Y_{24} \wedge \neg Y_{34}) \underline{\vee} (\neg Y_{14} \wedge Y_{24} \wedge \neg Y_{34}) \underline{\vee} (\neg Y_{14} \wedge \neg Y_{24} \wedge Y_{34})$$

$$W_{24} \Leftrightarrow (Y_{14} \wedge Y_{24} \wedge \neg Y_{34}) \underline{\vee} (\neg Y_{14} \wedge Y_{24} \wedge Y_{34})$$

$$W_{34} \Leftrightarrow Y_{14} \wedge Y_{24} \wedge Y_{34}$$

Logic Propositions

$$0 \le C_j, V_j, V_t^T, n_i, B_i, T_{Li}, pt_{ij}, N_j^{EQ}, pty_{itj};\ YEX_{tj}, Y_{tj}, YC_{cj}, W_{lj} \in \{true, false\}$$

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Proposed Algorithm for Nonconvex GDP

Step 0 — Nonconvex MINLP — OA *(Viswanathan and Grossmann, 1990)*

Z^U

Step 1 — Bound Contraction — *(Zamora and Grossmann, 1999)*

New Bound

Step 2 — BB with Y's, Update Z^L — Stop when $Z^L \geq Z^U$ — *(Lee and Grossmann, 2000)*

When solution is Integral

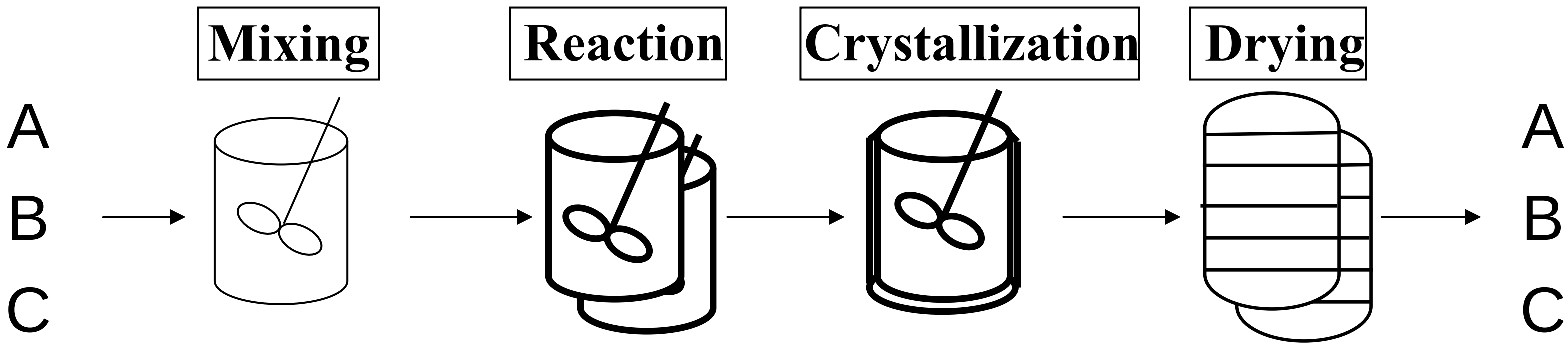
Add Integer Cut

Step 3 — Spatial BB, Update Z^U — Fixed Y's — *(Quesada and Grossmann, 1995)*

Upper Bound Solution

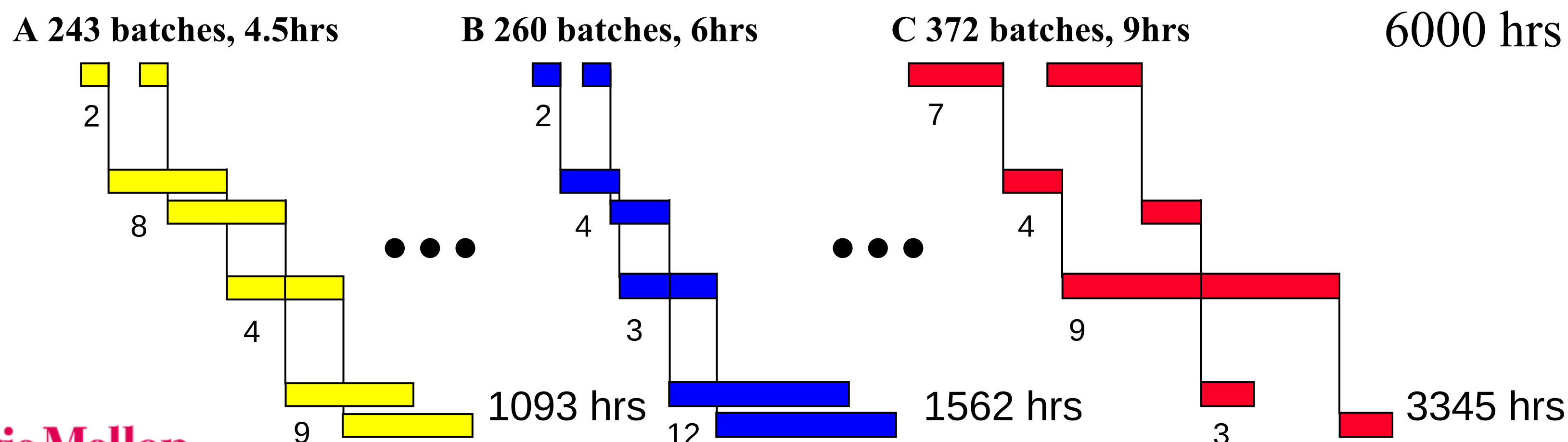
Cost = \$ 277,928 (by GAMS/DICOPT++)

- **Use 4 Stages (6 units) without Storage Tank**



$j = 1$ $\quad$ $j = 2$ $\quad$ $j = 4$ $\quad$ $j = 5$

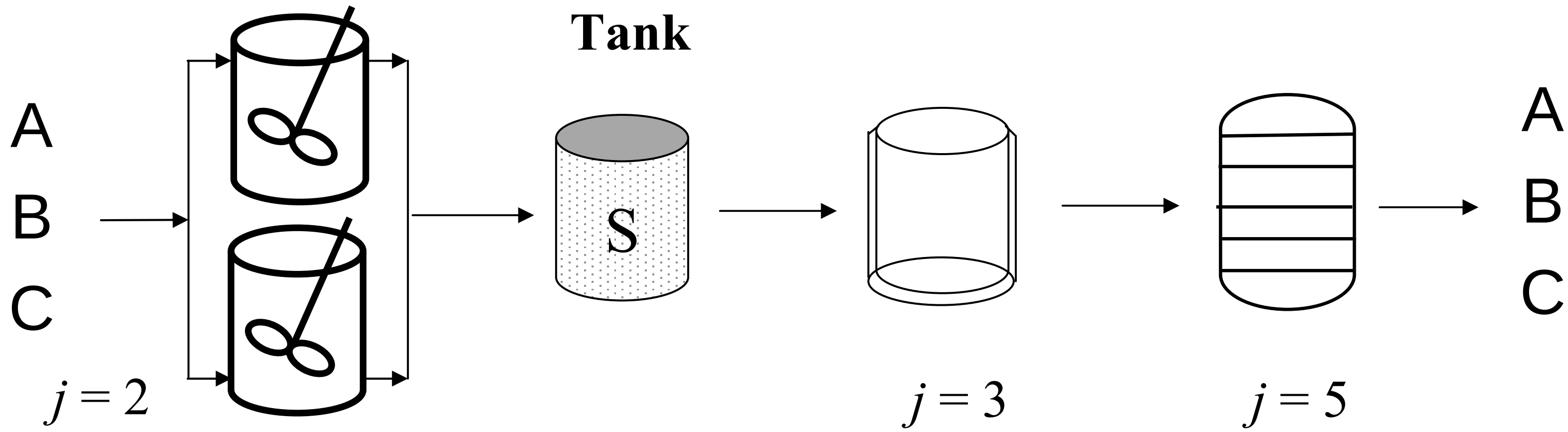
V_1 = 4,842 L $\quad$ **V_2 = 2,881 L** $\quad$ **V_4 = 2,469 L** $\quad$ **V_5 = 8,071 L**



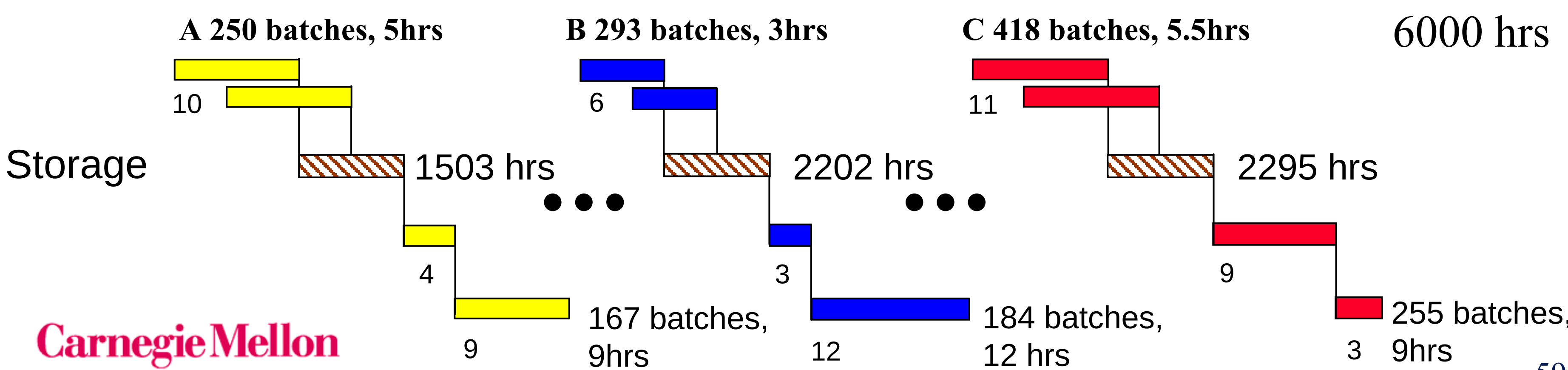
Optimal Solution: Multiproduct Batch Plant

- **Global optimal cost = \$ 264,887 (5% improvement)**
- **3 Stages + 1 storage tank (5 units)** ***(43 nodes, 48 sec)***

Mixing | Reaction   **Storage Tank**   **Crystallization**   **Drying**



V_2 = 4,309 L VST_2 = 4,800 L V_3 = 3,600 L V_5 = 11,753 L



Carnegie Mellon

Global Optimization of Bilinear Generalized Disjunctive Programs

Juan Ruiz

$$\begin{aligned}
&Min\ \ Z = \boxed{f(x)} + \sum_{k \in K} c_k && \longrightarrow \quad \textbf{Objective Function}\\
&s.t.\ \ \boxed{g(x)} \le 0 && \longrightarrow \quad \textbf{Global Constraints}\\
&\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ \boxed{r_{ik}(x)} \le 0 \\ c_k = \gamma_{ik} \end{bmatrix} && \longrightarrow \quad \textbf{Disjunctions}\ \ k \in K\\
&\Omega(Y) = True && \longrightarrow \quad \textbf{Logic Propositions}\\
&x \in R^n, c_k \in R, Y_{ik} \in \{True, False\} && \quad i \in D_k\ ,\ k \in K
\end{aligned}$$

Bilinearities

Bilinearities may lead to multiple local minima → Global Optimization techniques are required

Relaxation of Bilinear terms using McCormick envelopes leads to a LGDP → ***Improved relaxations for Linear GDP has recently been obtained (Sawaya & Grossmann, 2007)***

Guidelines for applying basic steps in Bilinear GDP

- Replace bilinear terms in GDP by McCormick convex envelopes (LGDP)
- Apply basic steps between those disjunctions with at least one variable in common.

  The more variables in common two disjunctions have the more the tightening can be expected
- If bilinearities are outside the disjunctions apply basic steps by introducing them in the disjunctions previous to the relaxation.

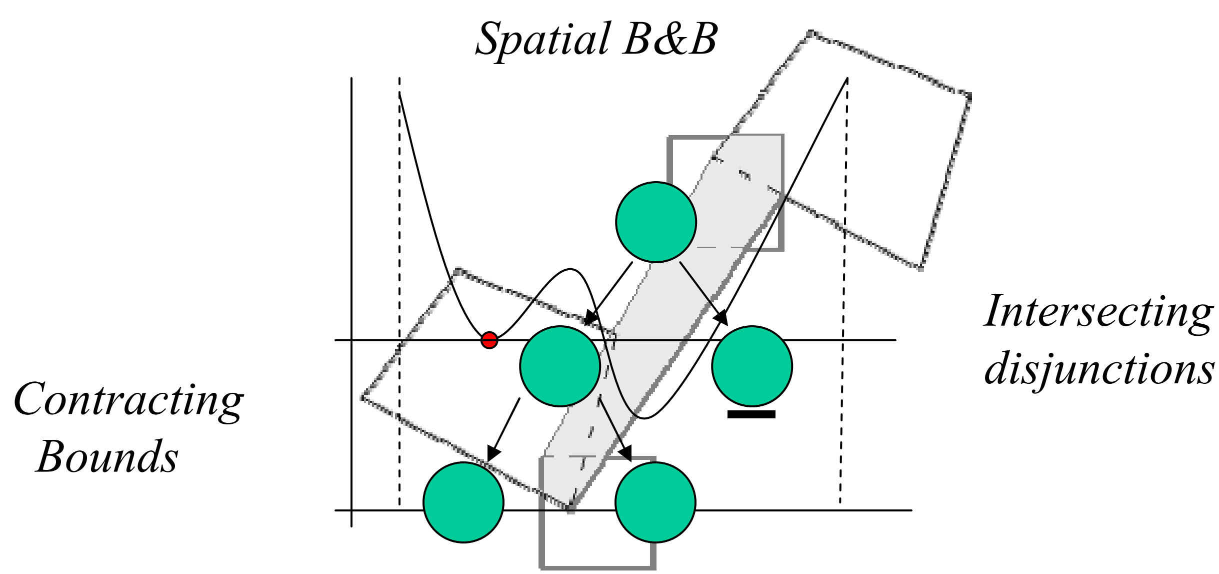
  If bilinearities are inside the disjunctions a smaller tightening effect is expected.
- A smaller increase in the size of the formulation is expected when basic steps are applied between improper disjunctions and proper disjunctions.

Methodology

Step 1: GDP reformulation (Apply basic steps following the rules presented)

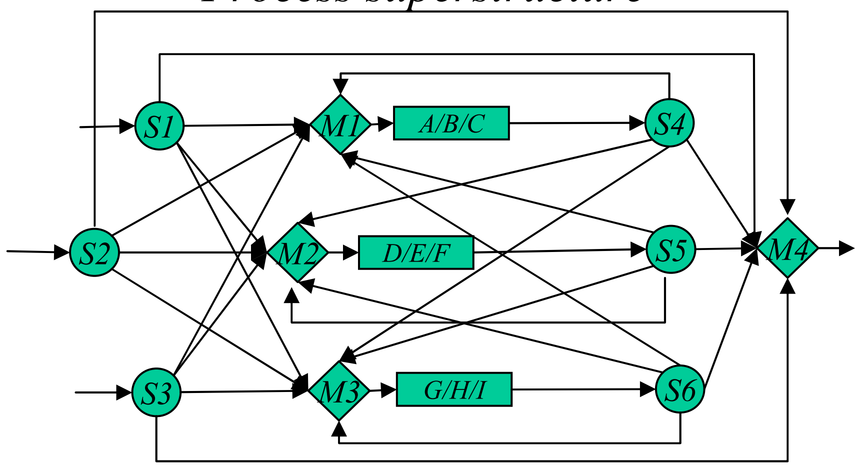
Step 2: Bound Contraction (Zamora & Grossmann, 1999)

Step 3: Branch and Bound Procedure (Lee & Grossmann, 2001)



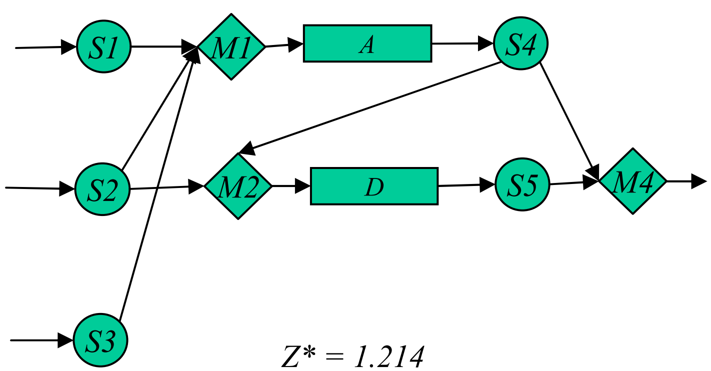
Case Study I: Water treatment network design

Process superstructure



N of cont. vars. : 114
N of disc. vars. : 9
N of bilinear terms: 36

Optimal structure



$Z^* = 1.214$

Generalized Disjunctive Program

$$Min\ Z = \sum_{k\in PU} CP_k$$

$s.t.$

$$f_k^j = \sum_{i\in M_k} f_i^j \qquad \forall j \quad k \in MU$$

$$\sum_{i\in S_k} f_i^j = f_k^j \qquad \forall j \quad k \in SU$$

$$\sum_{i\in S_k} \zeta_i^k = 1 \qquad k \in SU$$

$$\boxed{f_i^j = \zeta_i^k f_k^j} \qquad \forall j \quad i \in S_k \quad k \in SU$$

$$\bigvee_{h\in D_k} \begin{bmatrix} YP_k^h \\ f_i^j = \beta_k^{jh} f_{i'}^j, i \in OPU_k, i' \in IPU_k, \forall j \\ F_k = \sum_j f_i^j, i \in OPU_k \\ CP_k = \partial_{ik} F_k \end{bmatrix} \qquad k \in PU$$

$$0 \le \zeta_i^k \le 1 \qquad \forall j,k$$

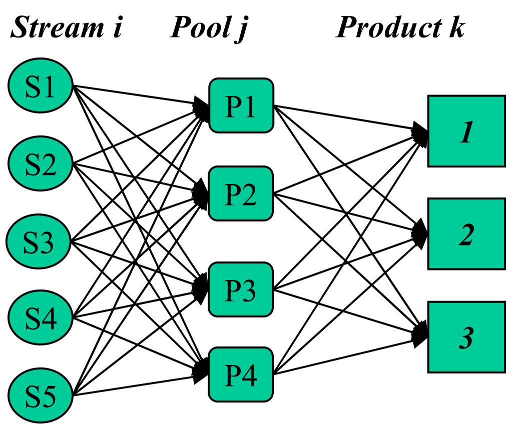
$$0 \le f_i^j, f_k^j \qquad \forall i,j,k$$

$$0 \le CP_k \qquad \forall k$$

$$YP_k^h \in \{true, false\} \qquad \forall h \in D_k \quad \forall k \in PU$$

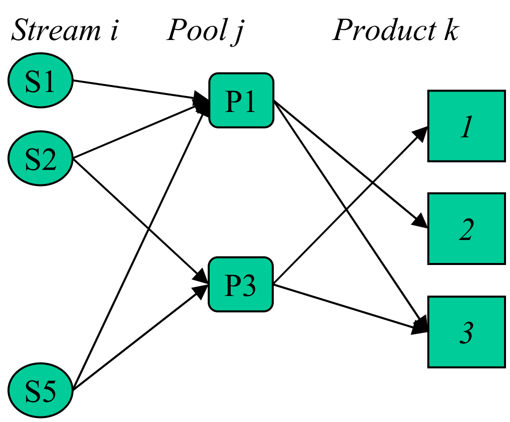
Case Study II: Pooling network design

Process superstructure



N of cont. vars. : 76
N of disc. vars. : 9
N of bilinear terms: 24

Optimal structure



$Z^* = -4.640$

Generalized Disjunctive Program

$$Min\ Z = \sum_{j\in J} CP_j + \sum_{i\in I} CST_i + \sum_{j\in J}\sum_{i\in I} c_{ij} \sum_{w\in W} f_{ijw} - \sum_{k\in K} d_k \sum_{j\in J}\sum_{w\in W} f_{jkw}$$

s.t.

$$\sum_{i\in I}\sum_{w\in W} f_{ijw} = \sum_{k\in K}\sum_{w\in W} f_{jkw} \qquad \forall j\in J$$

$$\sum_{j\in J}\sum_{w\in W} f_{jkw} - S_k = 0 \qquad \forall k\in K$$

$$f_{ijw} = \lambda_{iw} \sum_{w'\in W} f_{ijw'} \qquad \forall i\in I, \forall j\in J, \forall w\in W$$

$$\sum_{j\in J} f_{jkw} - Z_{kw} \sum_{j\in J}\sum_{w'\in W} f_{jkw'} = 0 \qquad \forall k\in K, \forall w\in W$$

$$\begin{bmatrix} YST_i \\ f^{lo} \le \sum_{j\in J}\sum_{w\in W} f_{ijw} \\ CST_i = \alpha_i \end{bmatrix} \vee \begin{bmatrix} \neg YST_i \\ f_{ijw} = 0 \\ CST_i = 0 \end{bmatrix} \qquad \forall i\in I$$

$$\begin{bmatrix} YP_j \\ f^{lo} \le \sum_{i\in I}\sum_{w\in W} f_{ijw} \\ \sum_{k\in K} f_{jkw} = \sum_{i\in I} f_{ijw}, \forall w\in W \\ \boxed{f_{jkw} = \zeta_j^{\,k} \sum_{i\in I} f_{ijw}}, \forall w\in W, k\in K \\ \sum_{k\in K} \zeta_j^{\,k} = 1 \\ CP_j = \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg YP_j \\ f_{ijw} = 0, \forall i\in I, w\in W \\ f_{jkw} = 0, \forall k\in K, w\in W \\ CP_j = 0 \end{bmatrix} \qquad \forall j\in J$$

$$0 \le \zeta_j^{\,k} \le 1; 0 \le f_{jkw}, f_{ijw} \le f^{up}$$

$$0 \le CST_i, CP_j; YST_i, YP_j \in \{true, false\}$$

Performance

		Global Optimization Technique using Lee & Grossmann relaxation	*Global Optimization Technique using proposed relaxation*	*Relative Improvement*
Example 1	**Initial Lower Bound**	**400.66**	**499.86**	**24.90%**
	Bound contraction			**99.7%**
	Nodes	**399**	**204**	**51%**

		Global Optimization Technique using Lee & Grossmann relaxation	*Global Optimization Technique using proposed relaxation*	*Relative Improvement*
Example 2	**Initial Lower Bound**	**-5515**	**-5468**	**0.90%**
	Bound contraction			**8%**
	Nodes	**748**	**683**	**9%**

Conclusions

GDP modeling framework

- Provides a logic-based framework for discrete-continuous optimization
- big-M and convex hull alternative formulations different relaxations
- Solution methods: reformulation, branch and bound, decomposition

Unified Linear GDP with Disjunctive Programming

- Developed DP equivalent formulation for GDP
- Developed a family of MIP reformulations for GDP
- Developed a hierarchy of relaxations for GDP
- Numerical results have shown great improvement in lower bound for strip packing problem

Nonconvex GDPs

- Spatial branch and bound methods can be developed
- Tighter lower bounds can be obtained in bilinear problems by applying basic steps

Open Cyberinfrastructure for Mixed-integer Nonlinear Programming: Collaboration and Deployment via Virtual Environments

CMU: Grossmann, Biegler, Belotti, Cornuejols, Margot, Ruiz, Sahinidis
IBM: Lee, Wächter

General Goals

***(a)** Create a library of optimization problems in different application areas in which one or several alternative models are presented with their derivation. In addition, each model has one or several instances that can serve to test various algorithms.*

***(b)** Provide a mechanism for researchers and users to contribute towards the creation of the library of optimization problems.*

***(c)** Provide a forum of discussion for algorithm developers and application users where alternative formulations can be discussed as well as performance and comparison of algorithms.*

***(d)** Provide information on MINLP tutorials and bibliography to disseminate this information.*

Major emphasis

Collect optimization problems in which alternative model formulations are documented with corresponding computational results (*engineering, finance, operations management, biology*)