

# Fundamentals of Theory and Practice of Mixed Integer Non Linear Programming

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[http://www.lix.polytechnique.fr/~dambrosio/teaching/STOR-i/stor-i\\_2019.php](http://www.lix.polytechnique.fr/~dambrosio/teaching/STOR-i/stor-i_2019.php)

- 1 Recap
  - What is a MINLP?
  - Exact reformulations
  - Relaxations
- 2 Example: Pooling Problem
- 3 Methods for convex MINLPs
- 4 Global Optimization methods
  - Multistart
  - Spatial Branch-and-Bound
    - Standard form
    - Convexification
    - Expression trees
    - Variable ranges
    - Bounds tightening
    - Reformulation Linearization Technique (RLT)

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# Recap: What is a MINLP?

(MINLP)

$$\begin{aligned} \min f(x, y) \\ g_i(x, y) &\leq 0 \quad \forall i = 1, \dots, m \\ x &\in X \\ y &\in Y \end{aligned}$$

where  $f(x, y) : \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $g_i(x) : \mathbb{R}^n \rightarrow \mathbb{R} \forall i, \dots, m$ ,  $X \subseteq \mathbb{R}^{n_1}$ ,  $Y \subseteq \mathbb{N}^{n_2}$ , and  $n = n_1 + n_2$ .

Hp.  $f$  and  $g$  are twice continuously differentiable functions.

# Recap: Exact reformulations

(MINLP')

$$\min h(w, z) \tag{1}$$

$$p_i(w, z) \leq 0 \quad \forall i = 1, \dots, r \tag{2}$$

$$w \in W \tag{3}$$

$$z \in Z \tag{4}$$

where  $h(w, z) : \mathbb{R}^q \rightarrow \mathbb{R}$ ,  $p_i(w, z) : \mathbb{R}^q \rightarrow \mathbb{R} \forall i = 1, \dots, r$ ,  $W \subseteq \mathbb{R}^{q_1}$ ,  $Z \subseteq \mathbb{R}^{q_2}$  and  $q = q_1 + q_2$ .

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The formulation (MINLP') is an **exact reformulation** of (MINLP) if

- $\forall (w', z')$  satisfying (2)-(4),  $\exists (x', y')$  feasible solution of (MINLP) s.t.  $\phi(w', z') = (x', y')$
- $\phi$  is efficiently computable
- $\forall (w', z')$  global solution of (MINLP'), then  $\phi(w', z')$  is a global solution of (MINLP)
- $\forall (x', y')$  global solution of (MINLP), there is a  $(w', z')$  global solution of (MINLP')

# Recap: Exact reformulations

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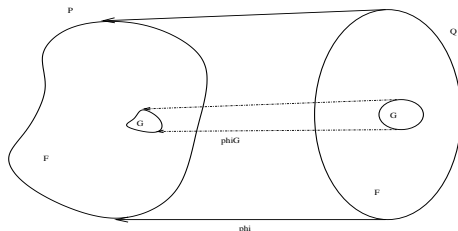
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# Recap: Relaxations

(rMINLP)

$$\begin{aligned} \min & \underline{f}(w, z) \\ & \underline{g}_i(w, z) \leq 0 \quad \forall i = 1, \dots, r \\ & w \in W \\ & z \in Z \end{aligned}$$

where  $X \subseteq W \subseteq \mathbb{R}^{q_1}$ ,  $Y \subseteq Z \subseteq \mathbb{Z}^{q_2}$ ,  $q_1 \geq n_1$ ,  $q_2 \geq n_2$ ,  $\underline{f}(w, z) \leq f(x, y)$   
 $\forall (x, y) \subseteq (w, z)$ , and  
 $\{(x, y) | g(x, y) \leq 0\} \subseteq \text{Proj}_{(x, y)} \{(w, z) | \underline{g}(w, z) \leq 0\}$ .

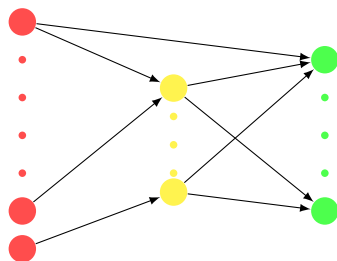
Examples:

- continuous relaxation: when  $(w, z) \in \mathbb{R}^n$ ,  $W = X$ ,  
 $\underline{f}(x, y) = f(x, y)$ ,  $\underline{g}(x, y) = g(x, y)$
- linear relaxation: when  $q = n$ ,  $W = X$ ,  $Z = Y$ ,  $\underline{f}(w, z)$  and  $\underline{g}(w, z)$   
are linear
- convex relaxation: when  $q = n$ ,  $W = X$ ,  $Z = Y$ ,  $\underline{f}(w, z)$  and  
 $\underline{g}(w, z)$  are convex



# Example: Pooling Problem

Inputs  $I$       Pools  $L$       Outputs  $J$



- Nodes  $N = I \cup L \cup J$
- Arcs  $A$   
 $(i, j) \in (I \times L) \cup (L \times J) \cup (I \times J)$   
on which materials flow
- Material attributes:  $K$
- Arc capacities:  $u_{ij}, (i, j) \in A$
- Node capacities:  $C_i, i \in N$
- **Attribute** requirements  
 $\alpha_{kj}, k \in K, j \in J$

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- different **specifications**: e.g., sulphur/carbon concentrations or physical properties such as density, octane number, ...
- wastewater treatment, e.g., Karuppiah and Grossmann (2006)
- Formally introduced by **Haverly (1978)**
- Alfaki and Haugland (2012) formally proved it is strongly **NP-hard**

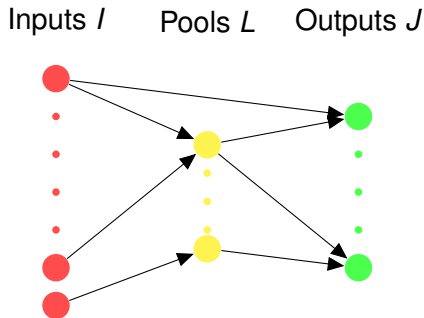
# Example: Pooling Problem

## “Simple” constraints

Variables  $x_{ij}$  for flow on arcs

Flow balance constraints at pools:

$$\sum_{i \in I_l} x_{il} - \sum_{j \in J_l} x_{lj} = 0, \quad \forall l \in L$$



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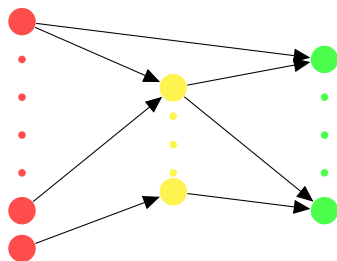
Capacity constraints:

$$\sum_{j \in J_i} x_{ij} + \sum_{l \in L_i} x_{il} \leq C_i, \quad \forall i \in I$$

$$\sum_{j \in J_l} x_{lj} \leq C_l, \quad \forall l \in L$$

$$\sum_{i \in I_j} x_{ij} + \sum_{l \in L_j} x_{lj} \leq C_j, \quad \forall j \in J$$

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## “Complicating” constraints

- Inputs have associated attribute concentrations  $\lambda_{ki}$ ,  $k \in K, i \in I$
  - Concentration of attribute in pool is the weighted average of the concentrations of its inputs.
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- **P-formulation** (Haverly 78):

Keep track of concentration  $p_{kl}$  of attribute  $k$  in pool  $l$

- **Q-formulation** (Ben-Tal et al. 94):

Variables  $q_{il}$  for proportion of flow into pool  $l$  coming from input  $i$

# Example: Pooling Problem

## P-formulation

$$\sum_{j \in J_i} x_{ij} + \sum_{l \in L_i} x_{il} \leq C_i, \quad \forall i \in I$$

$$\sum_{j \in J_l} x_{lj} \leq C_l, \quad \forall l \in L$$

$$\sum_{i \in I_j} x_{ij} + \sum_{l \in L_j} x_{lj} \leq C_j, \quad \forall j \in J$$

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$$\sum_{i \in I_l} x_{il} - \sum_{j \in J_l} x_{lj} = 0, \quad \forall l \in L$$

$$p_{kl} = \frac{\sum_{i \in I_l} \lambda_{ki} x_{il}}{\sum_{i \in J_l} x_{lj}} \quad \forall k \in K, l \in L$$

$$\frac{\sum_{i \in I_j} \lambda_{ki} x_{ij} + \sum_{l \in L_j} p_{kl} x_{lj}}{\sum_{i \in I_j \cup L_j} x_{ij}} \leq \alpha_{kj}, \quad \forall k \in K, j \in J$$

# Example: Pooling Problem

## P-formulation

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$$\sum_{i \in I_l} x_{il} - \sum_{j \in J_l} x_{lj} = 0, \quad \forall l \in L$$

$$\mathbf{p}_{kl} \sum_{i \in J_l} x_{ij} = \sum_{i \in I_l} \lambda_{ki} x_{il} \quad \forall k \in K, l \in L$$

$$\sum_{i \in I_j} \lambda_{ki} x_{ij} + \sum_{l \in L_j} \mathbf{p}_{kl} x_{lj} \leq \alpha_{kj} \sum_{i \in I_j \cup L_j} x_{ij}, \quad \forall k \in K, j \in J$$

# Example: Pooling Problem

## Q-formulation

$$x_{il} = q_{il} \sum_{j \in J_l} x_{lj}, \quad \forall i \in I, l \in L_i$$

$$\sum_{i \in I_l} q_{il} = 1, \quad \forall l \in L$$

## Q-formulation

$$x_{il} = q_{il} \sum_{j \in J_l} x_{lj}, \quad \forall i \in I, l \in L_i$$

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- Attribute constraints

$$\sum_{i \in I_j} \lambda_{ki} x_{ij} + \sum_{l \in L_j} x_{lj} \left( \sum_{i \in I_l} \lambda_{ki} q_{il} \right) \leq \alpha_{kj} \sum_{i \in I_j \cup L_j} x_{ij}, \quad \forall k \in K, j \in J$$

# Example: Pooling Problem

## Q-formulation

$$\sum_{j \in J_i} x_{ij} + \sum_{l \in L_i} x_{il} \leq C_i, \quad \forall i \in I$$

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$$x_{il} - \mathbf{q}_{il} \sum_{j \in J_l} \mathbf{x}_{lj} = 0 \quad \forall i \in I, l \in L_i$$

$$\sum_{i \in I_l} \mathbf{q}_{il} = 1 \quad \forall l \in L$$

$$\sum_{i \in I_j} \lambda_{ki} x_{ij} + \sum_{l \in L_j} \mathbf{x}_{lj} \left( \sum_{i \in I_l} \lambda_{ki} \mathbf{q}_{il} \right) \leq \alpha_{kj} \sum_{i \in I_j \cup L_j} x_{ij}, \quad \forall k \in K, j \in J$$



# Example: Pooling Problem with binary vars

## From NLP to MINLP

- Decide whether to install pipes or not (0/1 decision)
- Associate a binary variable  $z_{ij}$  with each pipe (suppose for now on arcs from input to output)

Extra constraints:

$$\begin{aligned}x_{ij} &\leq \min(C_i, C_j)z_{ij} && \forall i \in I, j \in J_i \\z_{ij} &\in \{0, 1\} && \forall i \in I, j \in J_i\end{aligned}$$

## Objective Function

- Fixed cost for installing pipe

$$\min \sum_{i \in I} c_i \left( \sum_{l \in L_i} x_{il} + \sum_{j \in J_i} x_{ij} \right) - \sum_{j \in J} p_j \left( \sum_{i \in I_j} x_{ij} + \sum_{l \in L_j} x_{lj} \right) + \sum_{i \in I} \sum_{j \in J_i} f_{ij} z_{ij}$$

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# MINLP branch-and-bound with local NLP solver

Branch-and-bound algorithm: solve continuous (NLP) relaxation at each node of the search tree and branch on variables.

NLP solver used:

Local NLP solvers  $\rightarrow$  local optimum

No valid bound for nonconvex MINLPs.

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LB = 30

0

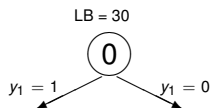
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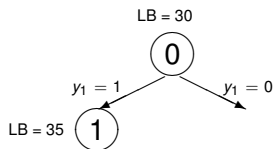
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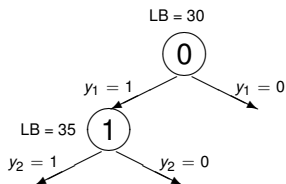
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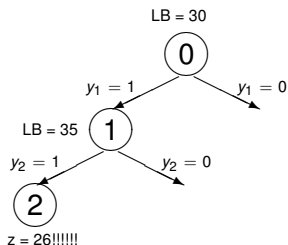
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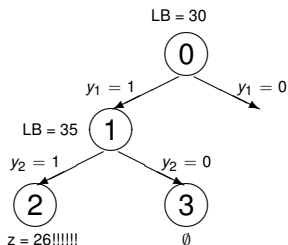
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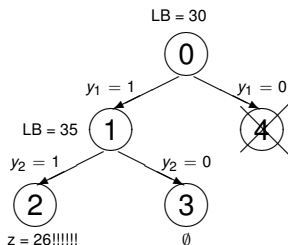
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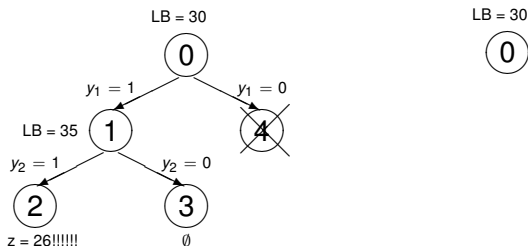
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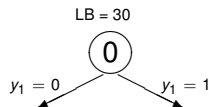
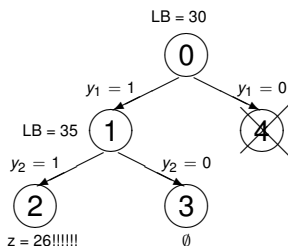
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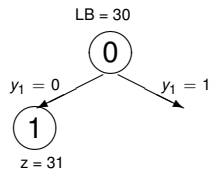
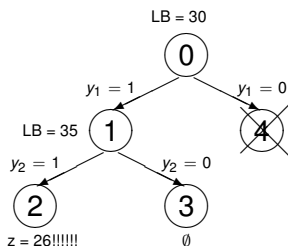
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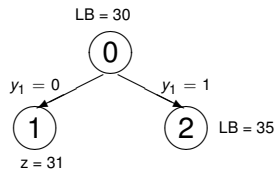
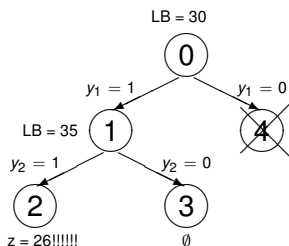
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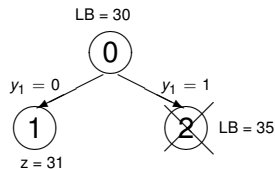
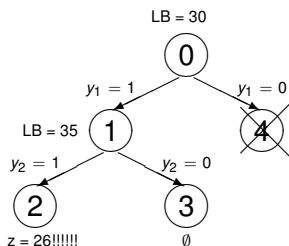
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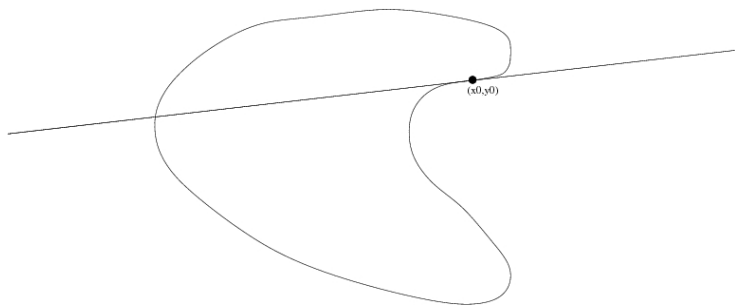


# Outer Approximation and nonconvex MINLPs

Several methods for convex MINLPs use **Outer Approximation** cuts (Duran and Grossman, 1986) which are not exact for nonconvex MINLPs.

$$g_i(x) \leq 0 \quad \rightarrow \quad g_i(x^k) + \nabla g_i(x^k)^T (x - x^k) \leq 0$$

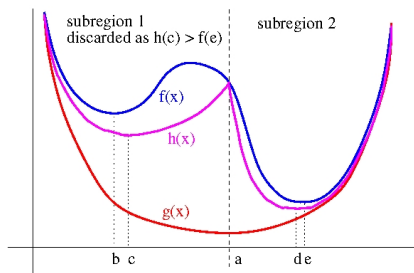
where  $\nabla g(x^k)$  is the Jacobian of  $g(x)$  evaluated at point  $(x^k)$ .





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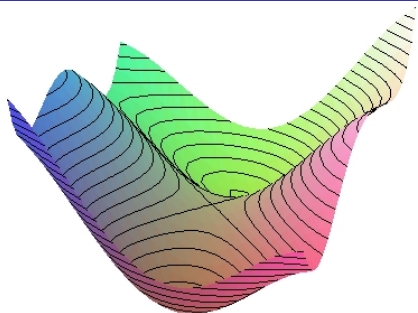
# Global Optimization methods



- objective function
- convex relaxation in whole space
- a: solution of convex relaxation in whole space
- b: local solution of objective function in whole space

## Exact

- “Exact” in continuous space:  
 *$\varepsilon$ -approximate (find solution within pre-determined  $\varepsilon$  distance from optimum in obj. fun. value)*
- For some problems, finite convergence to optimum ( $\varepsilon = 0$ )



## Heuristic

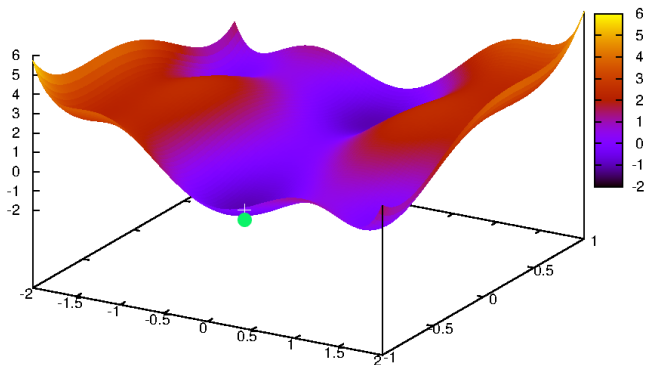
- Find solution with probability 1 in infinite time

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- The easiest GO method
  - 1:  $f^* = \infty$
  - 2:  $x^* = (\infty, \dots, \infty)$
  - 3: **while**  $\neg$  termination **do**
  - 4:    $x' = (\text{random}(), \dots, \text{random}())$
  - 5:    $x = \text{localSolve}(P, x')$
  - 6:   **if**  $f_P(x) < f^*$  **then**
  - 7:      $f^* \leftarrow f_P(x)$
  - 8:      $x^* \leftarrow x$
  - 9:   **end if**
  - 10: **end while**
- Termination condition: e.g. *repeat k times*

# Six-hump camelback function

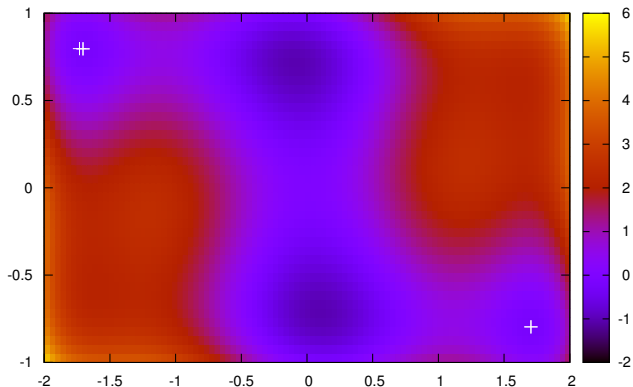
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Global optimum (COUENNE)

# Six-hump camelback function

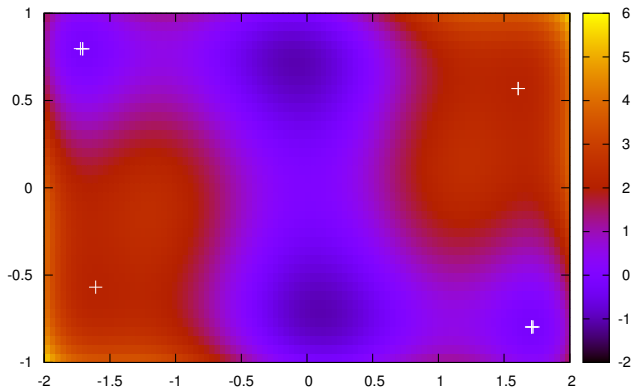
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT,  $k = 5$

# Six-hump camelback function

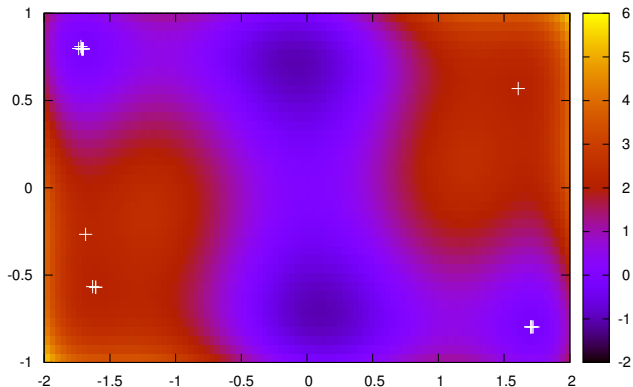
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT,  $k = 10$

# Six-hump camelback function

$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$

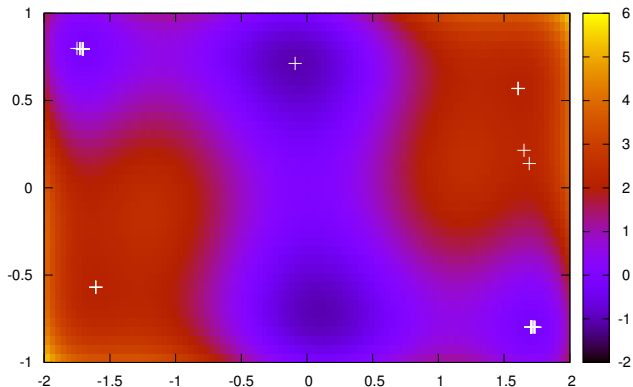


Multistart with IPOPT,  $k = 20$



# Six-hump camelback function

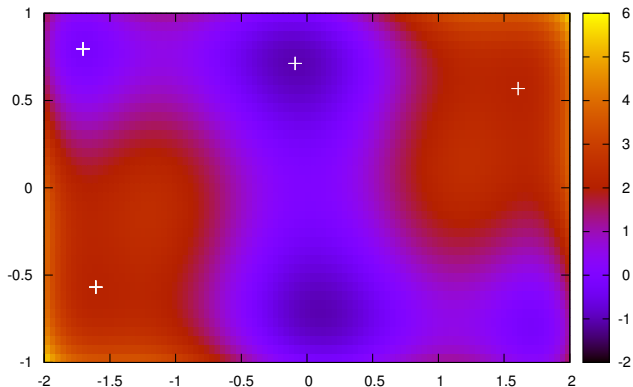
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT,  $k = 50$

# Six-hump camelback function

$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with SNOPT,  $k = 20$

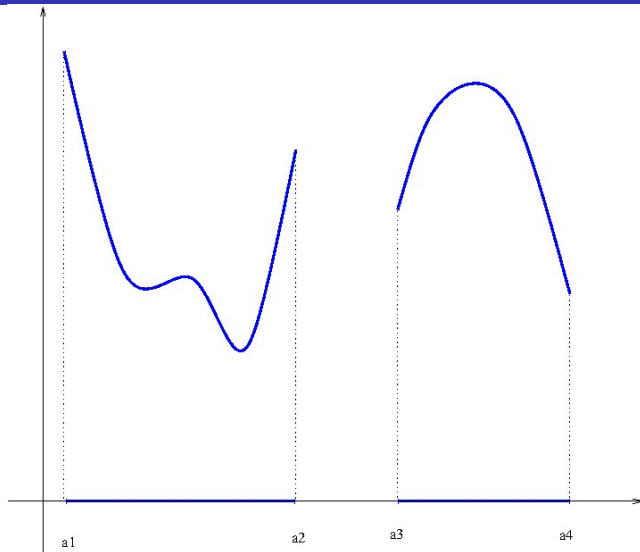
- 1 Recap
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Falk and Soland (1969) “An algorithm for separable nonconvex programming problems”.

20 years ago: first general-purpose “exact” algorithms for nonconvex MINLP.

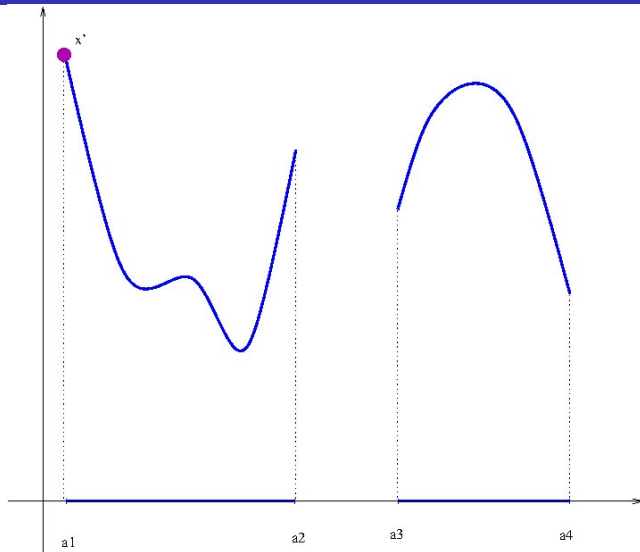
- Tree-like search
- Explores search space exhaustively but implicitly
- Builds a sequence of decreasing upper bounds and increasing lower bounds to the global optimum
- Exponential worst-case
- Only general-purpose “exact” algorithm for MINLP  
*Since continuous vars are involved, should say “ $\epsilon$ -approximate”*
- Like BB for MILP, but may branch on continuous vars  
*Done whenever one is involved in a nonconvex term*

# Spatial B&B: Example



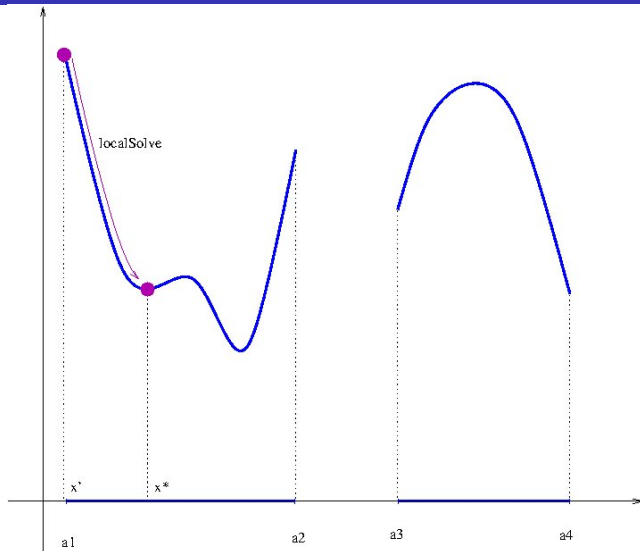
*Original problem P*

# Spatial B&B: Example



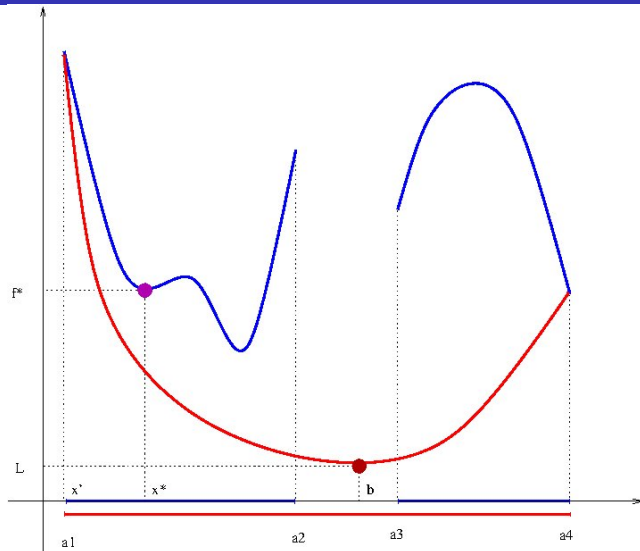
*Starting point  $x'$*

# Spatial B&B: Example



*Local (upper bounding) solution  $x^*$*

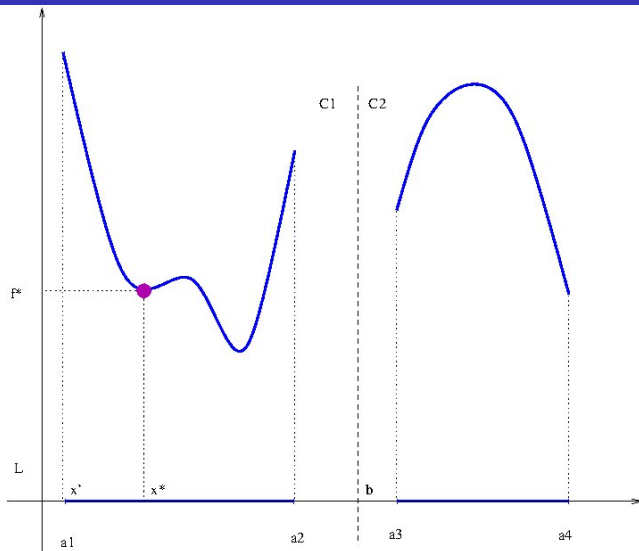
# Spatial B&B: Example



Convex relaxation (lower) bound  $\bar{f}$  with  $|f^* - \bar{f}| > \epsilon$

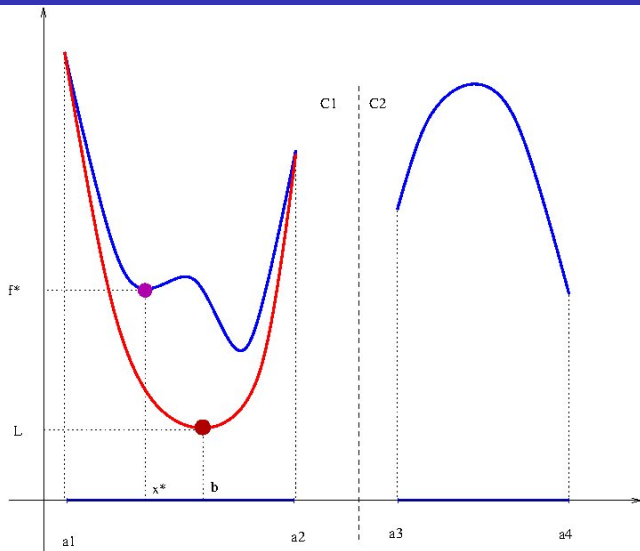


# Spatial B&B: Example



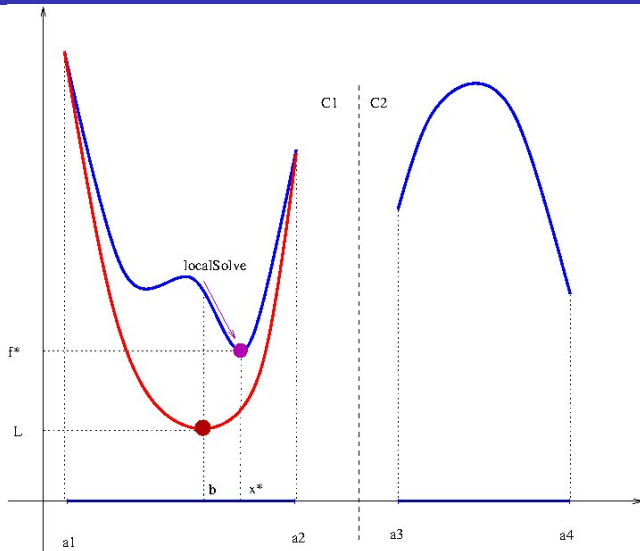
*Branch at  $x = \bar{x}$  into  $C_1, C_2$*

# Spatial B&B: Example



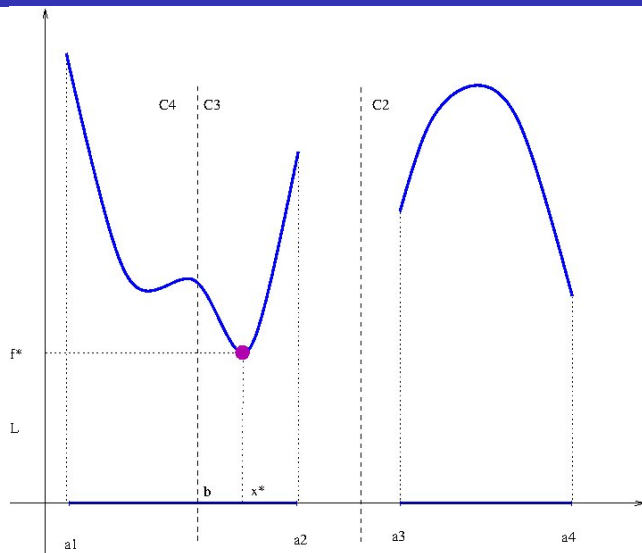
*Convex relaxation on  $C_1$ : lower bounding solution  $\bar{x}$*

# Spatial B&B: Example



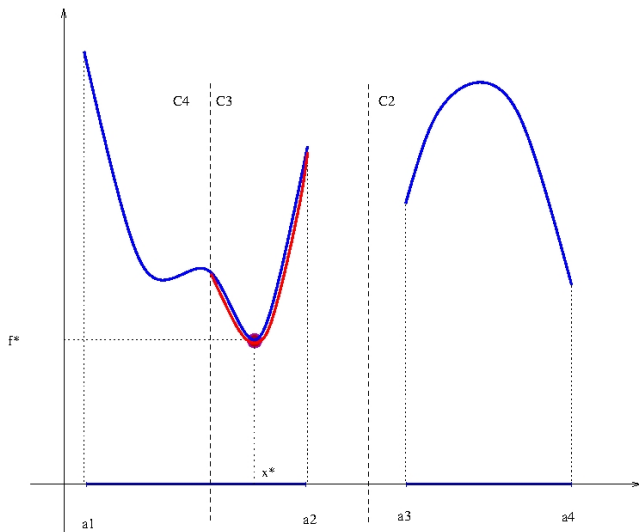
localSolve. from  $\bar{x}$ : new upper bounding solution  $x^*$

# Spatial B&B: Example



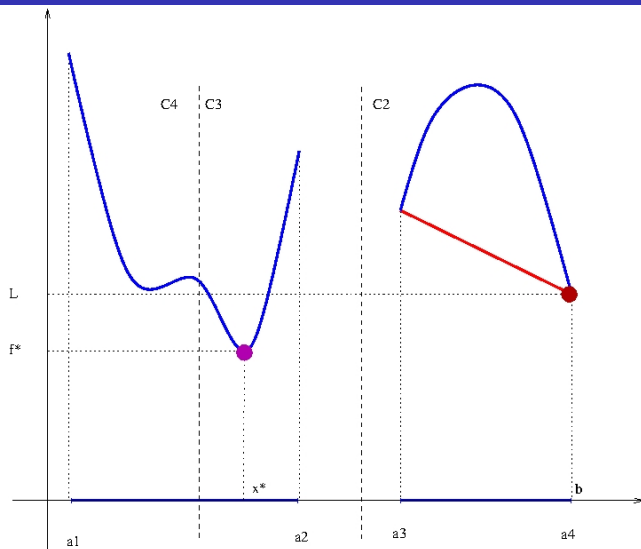
$|f^* - \bar{f}| > \varepsilon$ : branch at  $x = \bar{x}$

# Spatial B&B: Example



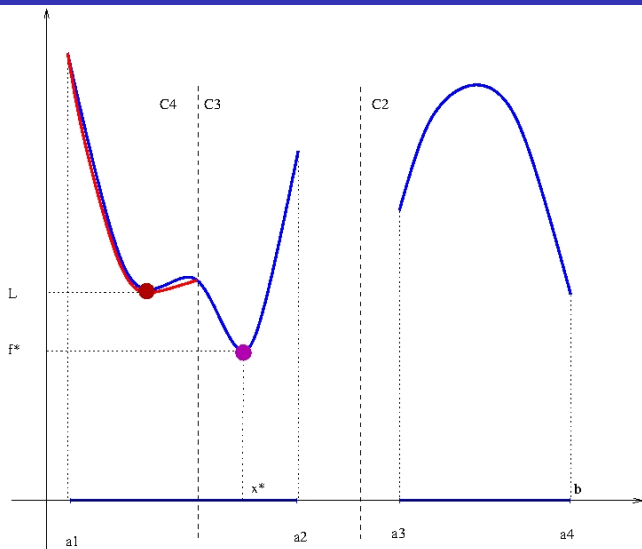
*Repeat on  $C_3$ : get  $\bar{x} = x^*$  and  $|f^* - \bar{f}| < \varepsilon$ , no more branching*

# Spatial B&B: Example



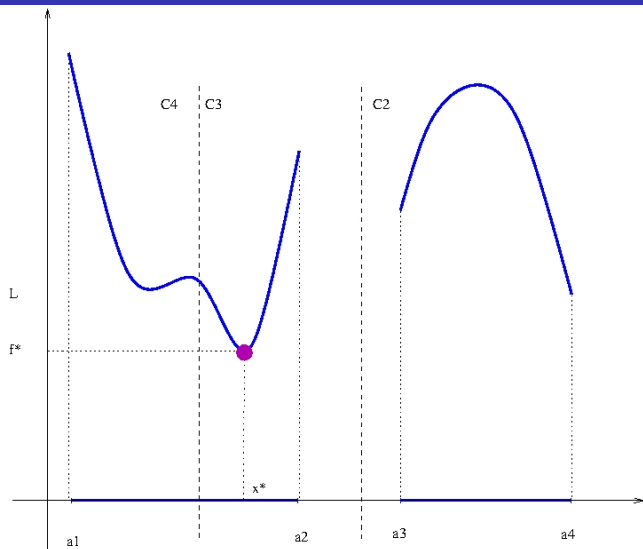
*Repeat on  $C_2$ :  $\bar{f} > f^*$  (can't improve  $x^*$  in  $C_2$ )*

# Spatial B&B: Example



Repeat on  $C_4$ :  $\bar{f} > f^*$  (can't improve  $x^*$  in  $C_4$ )

# Spatial B&B: Example



*No more subproblems left, return  $x^*$  and terminate*



# Spatial B&B: Pruning

- 1  $P$  was branched into  $C_1, C_2$
  - 2  $C_1$  was branched into  $C_3, C_4$
  - 3  $C_3$  was **pruned by optimality**  
( $x^* \in \mathcal{G}(C_3)$  was found)
  - 4  $C_2, C_4$  were **pruned by bound**  
(lower bound for  $C_2$  worse than  $f^*$ )
  - 5 No more nodes: whole space explored,  $x^* \in \mathcal{G}(P)$
- Search generates a tree
  - Suproblems are nodes
  - Nodes can be pruned by optimality, bound or **infeasibility** (when subproblem is infeasible)
  - Otherwise, they are branched

# Spatial B&B: General idea

Aimed at solving “factorable functions”, i.e.,  $f$  and  $g$  of the form:

$$\sum_h \prod_k f_{hk}(x, y)$$

where  $f_{hk}(x, y)$  are univariate functions  $\forall h, k$ .

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- Exact reformulation of MINLP so as to have “isolated basic nonlinear functions” (additional variables and constraints).

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- Relax (linear/convex) the basic nonlinear terms (library of envelopes/underestimators).

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- Exact reformulation of MINLP so as to have “isolated basic nonlinear functions” (additional variables and constraints).
- Relax (linear/convex) the basic nonlinear terms (library of envelopes/underestimators).
- Relaxation depends on variable bounds, thus branching potentially strengthen it.

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# Spatial B&B: exact reformulation to standard form

Consider a NLP for simplicity. Transform it in a standard form like:

$$\min c^T(x, w)$$

$$A(x, w) \leq b$$

$$w_{ij} = x_i \otimes x_j \quad \text{for suitable } i, j$$

$$x \in X$$

$$w \in W$$

where, for example,  $\otimes \in \{\text{sum, product, quotient, power, exp, log, sin, cos, abs}\}$  (Couenne).

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# Spatial B&B: convexification

Relax  $w_{ij} = x_i \otimes x_j \forall$  suitable  $i, j$  where  $\otimes \in \{\text{sum, product, quotient, power, exp, log, sin, cos, abs}\}$  such that:

$$w_{ij} \leq \text{overestimator}(x_i \otimes x_j)$$

$$w_{ij} \geq \text{underestimator}(x_i \otimes x_j)$$

Convex relaxation is not the tightest possible, but built automatically.

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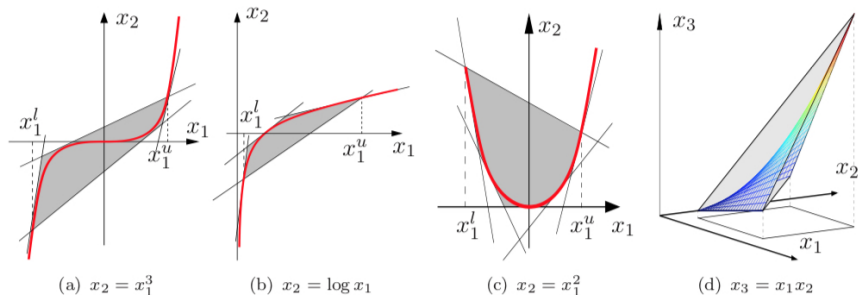
$$w_{ij} \leq \text{overestimator}(x_i \otimes x_j)$$

$$w_{ij} \geq \text{underestimator}(x_i \otimes x_j)$$

Convex relaxation is not the tightest possible, but built automatically.

- Underestimator/overestimator of convex/concave function: tangent cuts (OA)
- Odd powers or Trigonometric functions: separate intervals in which function is convex or concave and do as for convex/concave functions
- Product or Quotient: Mc Cormick relaxation

# Spatial B&B: Examples of Convexifications



P. Belotti, J. Lee, L. Liberti, F. Margot, A. Wächter, “Branching and bounds tightening techniques for non-convex MINLP”. *Optimization Methods and Software* 24(4-5): 597-634 (2009).

# Example: Standard Form Reformulation

$$\begin{aligned} \min \quad & x_1^2 + x_1 x_2 \\ & x_1 + x_2 \geq 1 \\ & x_1 \in [0, 1] \\ & x_2 \in [0, 1] \end{aligned}$$

# Example: Standard Form Reformulation

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becomes

$$\begin{aligned} \min \quad & w_1 + w_2 \\ & w_1 = x_1^2 \\ & w_2 = x_1 x_2 \\ & x_1 + x_2 \geq 1 \\ & x_1 \in [0, 1] \\ & x_2 \in [0, 1] \end{aligned}$$

# Example: .mod from Couenne

```
var x1 <= 1, >= 0;
```

```
var x2 <= 1, >= 0;
```

```
minimize of:
```

```
x1**2 + x1*x2;
```

```
subject to constraint:
```

```
x1 + x2 >= 1;
```

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```
var x1 <= 1, >= 0;  
var x2 <= 1, >= 0;  
  
minimize of:  
x1**2 + x1*x2;  
subject to constraint:  
x1 + x2 >= 1;
```

```
# Problem name: extended-aw.mod  
  
# original variables  
  
var x_0 >= 0 <= 1 default 0;  
var w_1 >= 0 <= 1 default 1;  
var w_2 >= 0 <= 1 default 0;  
var w_3 >= 0 <= 1 default 0;  
var w_4 >= 0 <= 2 default 0;  
  
# objective  
  
minimize obj: w_4;  
  
# aux. variables defined  
  
aux1: w_1 = (1-x_0);  
aux2: w_2 = (x_0**2);  
aux3: w_3 = (x_0*w_1);  
aux4: w_4 = (w_2+w_3);  
  
# constraints
```

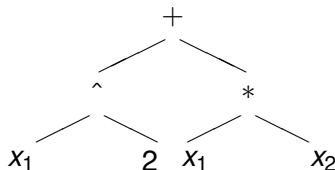
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## *Representation of objective $f$ and constraints $g$*

Encode mathematical expressions in trees or DAGs

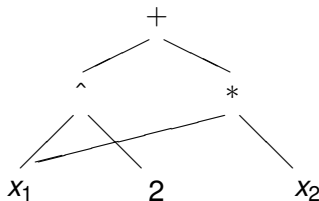
E.g.  $x_1^2 + x_1 x_2$ :



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- Crucial property for sBB convergence: **convex relaxation tightens as variable range widths decrease**
- convex/concave under/over-estimator constraints are (convex) functions of  $x^L, x^U$
- it makes sense to **tighten**  $x^L, x^U$  at the sBB root node (trading off speed for efficiency) and at each other node (trading off efficiency for speed)

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- In sBB we need to tighten variable bounds at each node
- Two methods:
  - Optimization Based Bounds Tightening (OBBT)
  - Feasibility Based Bounds Tightening (FBBT)

- **OBBT:**

for each variable  $x$  in  $P$  compute

- $\underline{x} = \min\{x \mid \text{conv. rel. constr.}\}$
- $\bar{x} = \max\{x \mid \text{conv. rel. constr.}\}$

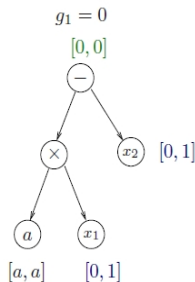
Set  $\underline{x} \leq x \leq \bar{x}$

# Bounds Tightening

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- **FBBT:**

**propagation of intervals up and down  
constraint expression trees, with tightening  
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Example:  $5x_1 - x_2 = 0$ .



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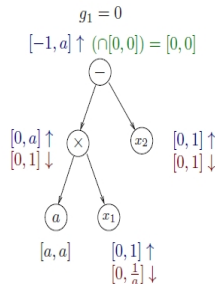
Example:  $5x_1 - x_2 = 0$ .

Up:  $\otimes: [5, 5] \times [0, 1] = [0, 5]$ ;  $\ominus: [0, 5] - [0, 1] = [-1, 5]$ .

Root node tightening:  $[-1, 5] \cap [0, 0] = [0, 0]$ .

Downwards:  $\otimes: [0, 0] + [0, 1] = [0, 1]$ ;

$x_1: [0, 1] / [5, 5] = [0, \frac{1}{5}]$





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    - **Reformulation Linearization Technique (RLT)**

- All nonlinear terms are quadratic monomials
- Aim to reduce gap between the problem and its convex relaxation
- $\Rightarrow$  replace quadratic terms with suitable linear constraints (fewer nonlinear terms to relax)
- Can be obtained by considering linear relations (called **reduced RLT constraints**) between original and linearizing variables

- For each  $k \leq n$ , let  $w_k = (w_{k1}, \dots, w_{kn})$
- Multiply  $Ax = b$  by each  $x_k$ , substitute linearizing variables  $w_k$ , get **reduced RLT constraint system** (RRCS)

$$\forall k \leq n (Aw_k = bx_k)$$

- $\forall i, k \leq n$  define  $z_{ki} = w_{ki} - x_i x_k$ , let  $z_k = (z_{k1}, \dots, z_{kn})$
- Substitute  $b = Ax$  in RRCS, get  $\forall k \leq n (A(w_k - x_k x) = 0)$ , i.e.  $\forall k \leq n (Az_k = 0)$ . Let  $B, N$  be the sets of basic and nonbasic variables of this system
- Setting  $z_{ki} = 0$  for each nonbasic variable implies that the RRCS is satisfied  $\Rightarrow$  It suffices to enforce quadratic constraints  $w_{ki} = x_i x_k$  for  $(i, k) \in N$  (replace those for  $(i, k) \in B$  with the linear RRCS)

# Example: pooling problem

## Q-formulation

$$\sum_{j \in J_i} x_{ij} + \sum_{l \in L_i} x_{il} \leq C_i, \quad \forall i \in I$$

$$\sum_{j \in J_l} x_{lj} \leq C_l, \quad \forall l \in L$$

$$\sum_{i \in I_j} x_{ij} + \sum_{l \in L_j} x_{lj} \leq C_j, \quad \forall j \in J$$

---

$$x_{il} - q_{il} \sum_{j \in J_l} x_{lj} = 0 \quad \forall i \in I, l \in L_i$$

$$\sum_{i \in I_l} q_{il} = 1 \quad \forall l \in L$$

$$\sum_{i \in I_j} \lambda_{ki} x_{ij} + \sum_{l \in L_j} x_{lj} \left( \sum_{i \in I_l} \lambda_{ki} q_{il} \right) \leq \alpha_{kj} \sum_{i \in I_j \cup L_j} x_{ij}, \quad \forall k \in K, j \in J$$

# Example: pooling problem

PQ-formulation by Sahinidis and Tawarmalani (2005).

Like Q-formulation but with extra (**redundant**) constraints:

- $x_{lj} \sum_{i \in I_l} q_{il} = x_{lj} \quad \forall l \in L, j \in J_l$
- $q_{il} \sum_{j \in J_l} x_{lj} \leq C_l q_{il} \quad \forall i \in I, l \in L_i$

# Example: pooling problem

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**One of the strongest known formulation!**

- Sherali, Alameddine, *A new reformulation-linearization technique for bilinear programming problems*, JOGO, 1991
- Falk, Soland, *An algorithm for separable nonconvex programming problems*, Manag. Sci. 1969.
- Horst, Tuy, *Global Optimization*, Springer 1990.
- Ryoo, Sahinidis, *Global optimization of nonconvex NLPs and MINLPs with applications in process design*, Comp. Chem. Eng. 1995.
- Adjiman, Floudas et al., *A global optimization method,  $\alpha$ BB, for general twice-differentiable nonconvex NLPs*, Comp. Chem. Eng. 1998.
- Smith, Pantelides, *A symbolic reformulation/spatial branch-and-bound algorithm for the global optimisation of nonconvex MINLPs*, Comp. Chem. Eng. 1999.
- Nowak, *Relaxation and decomposition methods for Mixed Integer Nonlinear Programming*, Birkhäuser, 2005.
- Belotti, et al., *Branching and bounds tightening techniques for nonconvex MINLP*, Opt. Meth. Softw., 2009.
- Vigerske, PhD Thesis: *Decomposition of Multistage Stochastic Programs and a Constraint Integer Programming Approach to Mixed-Integer Nonlinear Programming*, Humboldt-University Berlin, 2013.