Programmation Mathématique Avancée: Mixed Integer Non Linear Programming

Claudia D'Ambrosio

LIX, CNRS & École Polytechnique

MPRO – PMA

http://www.lix.polytechnique.fr/~dambrosio/teaching/MPRO/PMA-2024/pma-2024.php

Important Information

Exam starting at **09:30**

Outline

1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Recap: What is a MINLP?

(MINLP)

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

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

Hp. f and g are twice continuously differentiable functions.

Recap: Exact reformulations

(MINLP')

$$
\begin{aligned}
\min h(w,z) & & & (1)\\
p_i(w,z) & \leq 0 \quad \forall i = 1,\ldots,r & & (2)\\
w & \in W & & (3)\\
z & \in Z & & (4)
\end{aligned}
$$

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

Recap: Exact reformulations

(MINLP')

$$\min h(w,z) \tag{1}$$
$$p_i(w,z) \leq 0 \quad \forall i = 1,\dots,r \tag{2}$$
$$w \in W \tag{3}$$
$$z \in Z \tag{4}$$

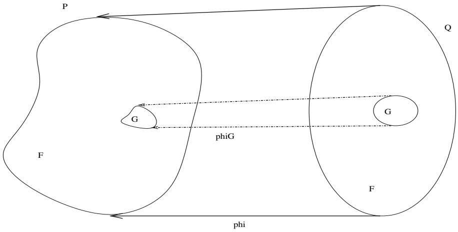
where $h(w,z) : \mathbb{R}^q \to \mathbb{R}$, $p_i(w,z) : \mathbb{R}^q \to \mathbb{R}\ \forall i = 1,\dots,r$, $W \subseteq \mathbb{R}^{q_1}$, $Z \subseteq \mathbb{N}^{q_2}$ and $q = q_1 + q_2$.
The formulation (MINLP') is an **exact reformulation** of (MINLP) if

- $\forall (w',z')$ satisfying (2)-(4), $\exists (x',y')$ feasible solution of (MINLP) s.t. $\phi(w',z') = (x',y')$
- ϕ 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')

(MINLP')

$$
\begin{aligned}
\min h(w,z) & & & (1)\\
p_i(w,z) &\le 0 \quad \forall i = 1,\ldots,r & & (2)\\
w &\in W & & (3)\\
z &\in Z & & (4)
\end{aligned}
$$

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



Recap: Relaxations

(rMINLP)

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

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 $\{(x,y)|g(x,y) \leq 0\} \subseteq \mathrm{Proj}_{(x,y)}\{(w,z)|\underline{g(w,z)} \leq 0\}$.

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

Outline

1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Pooling Problem

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**
- different **specifications**: e.g., sulphur/carbon concentrations or physical properties such as density, octane number, **...**

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**
- different **specifications**: e.g., sulphur/carbon concentrations or physical properties such as density, octane number, ...
- wastewater treatment, e.g., Karuppiah and Grossmann (2006)

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**
- 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)**

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**
- 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**

Pooling problem: Citations

- Haverly, *Studies of the behaviour of recursion for the pooling problem*, ACM SIGMAP Bulletin, 1978
- Adhya, Tawarmalani, Sahinidis, *A Lagrangian approach to the pooling problem*, Ind. Eng. Chem., 1999
- Audet et al., *Pooling Problem: Alternate Formulations and Solution Methods*, Manag. Sci., 2004
- Liberti, Pantelides, *An exact reformulation algorithm for large nonconvex NLPs involving bilinear terms*, JOGO, 2006
- Misener, Floudas, *Advances for the pooling problem: modeling, global optimization, and computational studies*, Appl. Comput. Math., 2009
- D'Ambrosio, Linderoth, Luedtke, *Valid inequalities for the pooling problem with binary variables*, IPCO, 2011
- Tawarmalani and Sahinidis. Convexification and global optimization in continuous and mixed-integer nonlinear programming: theory, algorithms, software, and applications, Ch. 9. Kluwer Academic Publishers, 2002.

Motivating Application

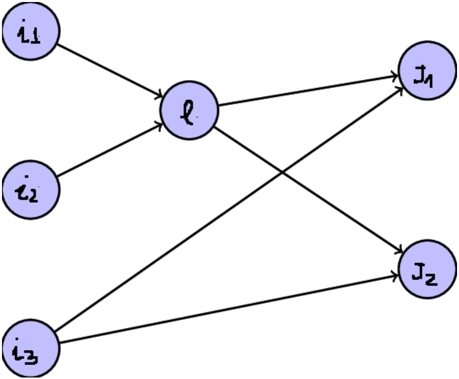


Figure: The Haverly Instance. Source: Alfaki.

Motivating Application

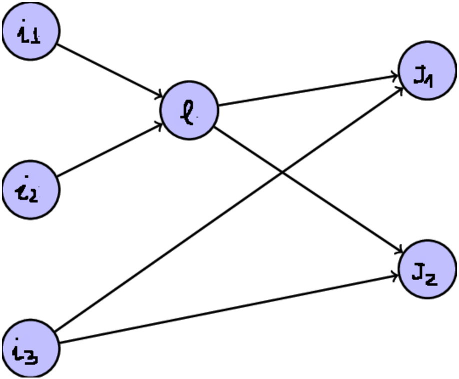


Figure: The Haverly Instance. Source: Alfaki.

demand = (100,200); unit profit = (9, 15)

Motivating Application

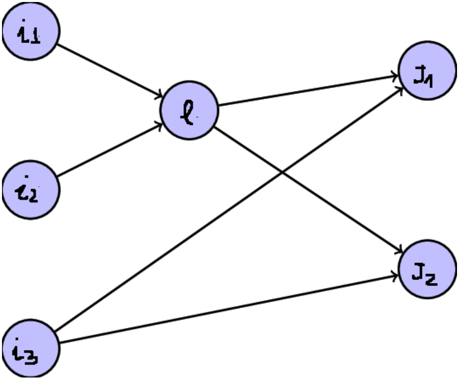


Figure: The Haverly Instance. Source: Alfaki.

demand = (100,200); unit profit = (9, 15)
cost = (6, 16, 10)

Motivating Application

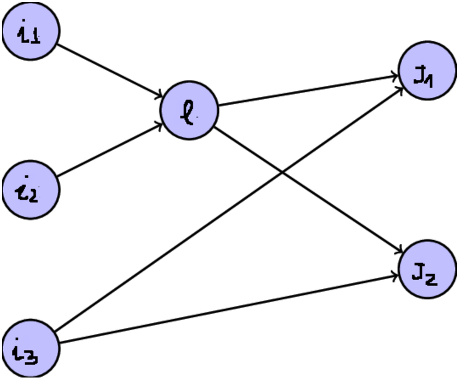


Figure: The Haverly Instance. Source: Alfaki.

demand = (100,200); unit profit = (9, 15)
cost = (6, 16, 10)
sulphur concentration = (3, 1, 2)

Motivating Application

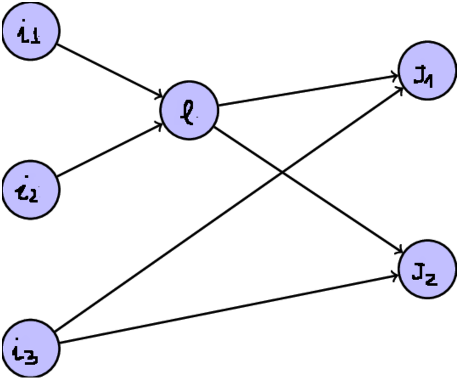


Figure: The Haverly Instance. Source: Alfaki.

demand = (100,200); unit profit = (9, 15)
cost = (6, 16, 10)
sulphur concentration = (3, 1, 2)
sulphur c. max = (2.5, 1.5)

Motivating Application

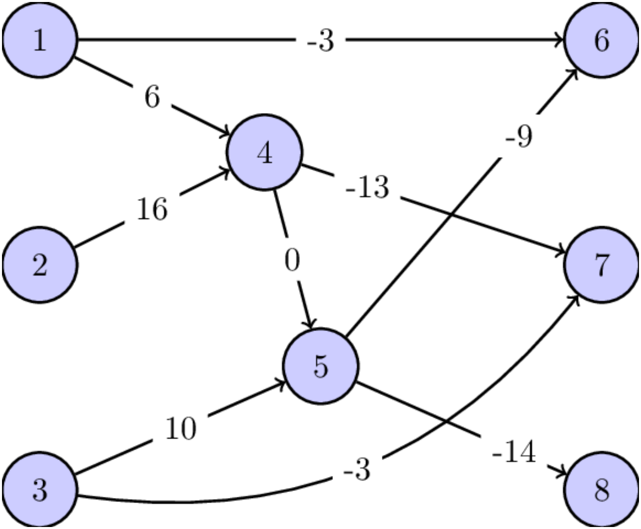


Figure: Audet et al.'s Instance. Source: Alfaki.

Motivationng Application

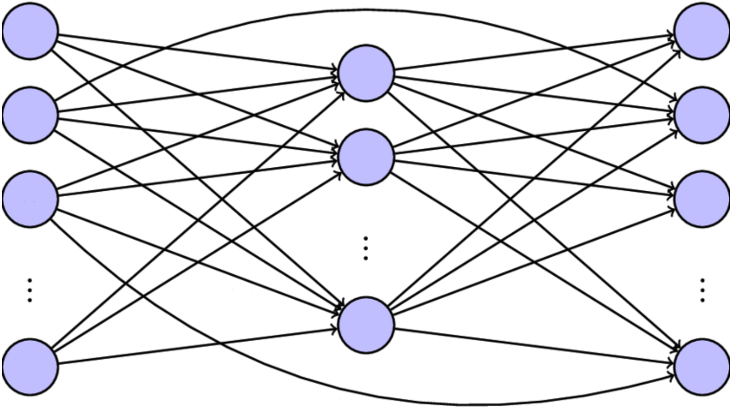


Figure: A generic Instance. Source: Alfaki.

Motivating Application

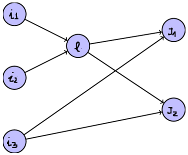


Figure: The Haverly Instance. Source: Alfaki.

Motivating Application

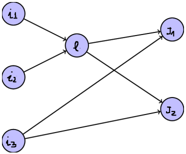


Figure: The Haverly Instance. Source: Alfaki.

$$\max 9x_{l,j_1} + 9x_{i_3,j_1} + 15x_{l,j_2} + 15x_{i_3,j_2} - 6x_{i_1,l} - 16x_{i_2,l} - 10x_{i_3,j_1} - 10x_{i_3,j2}$$

Motivating Application

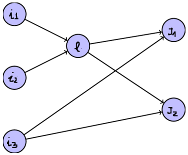


Figure: The Haverly Instance. Source: Alfaki.

$$\max 9x_{l,j_1} + 9x_{i_3,j_1} + 15x_{l,j_2} + 15x_{i_3,j_2} - 6x_{i_1,l} - 16x_{i_2,l} - 10x_{i_3,j_1} - 10x_{i_3,j2}$$

$$x_{l,j_1} + x_{i_3,j_1} \leq 100$$
$$x_{l,j_2} + x_{i_3,j_2} \leq 200$$

Motivating Application

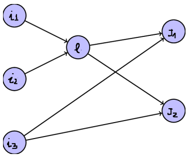


Figure: The Haverly Instance. Source: Alfaki.

$$\max 9x_{l,j_1} + 9x_{i_3,j_1} + 15x_{l,j_2} + 15x_{i_3,j_2} - 6x_{i_1,l} - 16x_{i_2,l} - 10x_{i_3,j_1} - 10x_{i_3,j2}$$

$$x_{l,j_1} + x_{i_3,j_1} \le 100$$
$$x_{l,j_2} + x_{i_3,j_2} \le 200$$

$$x_{i_1,l} + x_{i_2,l} = x_{l,j_1} + x_{l,j_2}$$

Motivating Application

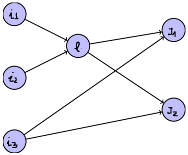


Figure: The Haverly Instance. Source: Alfaki.

$$\max 9x_{l,j_1} + 9x_{i_3,j_1} + 15x_{l,j_2} + 15x_{i_3,j_2} - 6x_{i_1,l} - 16x_{i_2,l} - 10x_{i_3,j_1} - 10x_{i_3,j2}$$

$$x_{l,j_1} + x_{i_3,j_1} \leq 100$$
$$x_{l,j_2} + x_{i_3,j_2} \leq 200$$

$$x_{i_1,l} + x_{i_2,l} = x_{l,j_1} + x_{l,j_2}$$

$$p_l x_{l,j_1} + 2x_{i_3,j_1} \leq 2.5(x_{l,j_1} + x_{i_3,j_1})$$
$$p_l x_{l,j_2} + 2x_{i_3,j_2} \leq 1.5(x_{l,j_2} + x_{i_3,j_2})$$

Motivating Application

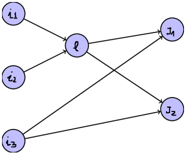


Figure: The Haverly Instance. Source: Alfaki.

$$\max 9x_{l,j_1} + 9x_{i_3,j_1} + 15x_{l,j_2} + 15x_{i_3,j_2} - 6x_{i_1,l} - 16x_{i_2,l} - 10x_{i_3,j_1} - 10x_{i_3,j2}$$

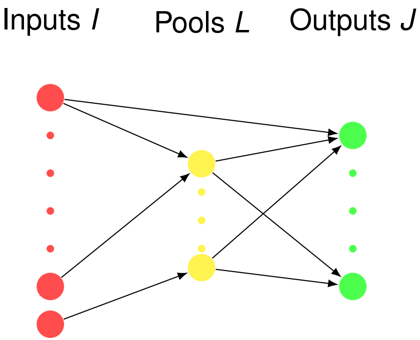
$$x_{l,j_1} + x_{i_3,j_1} \leq 100$$
$$x_{l,j_2} + x_{i_3,j_2} \leq 200$$

$$x_{i_1,l} + x_{i_2,l} = x_{l,j_1} + x_{l,j_2}$$

$$p_l x_{l,j_1} + 2x_{i_3,j_1} \leq 2.5(x_{l,j_1} + x_{i_3,j_1})$$
$$p_l x_{l,j_2} + 2x_{i_3,j_2} \leq 1.5(x_{l,j_2} + x_{i_3,j_2})$$

$$p_l(x_{l,j_1} + x_{l,j_2}) = 3x_{i_1,l} + x_{i_2,l}$$

Pooling Problem



- 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
  α_{kj}, $k \in K, j \in J$

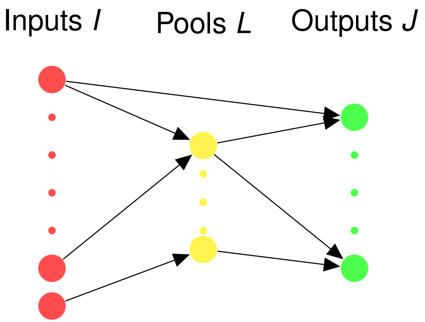
Example: Pooling Problem

“Simple” constraints

Variables x_{ij} for flow on arcs

Flow balance constraints at pools:

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



Example: Pooling Problem

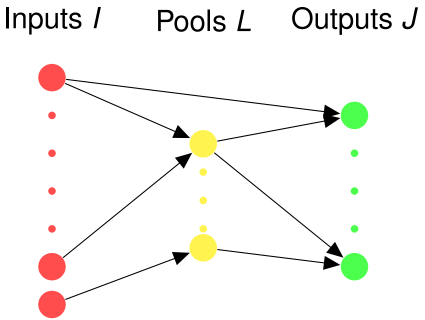
"Simple" constraints

Variables x_{ij} for flow on arcs

Flow balance constraints at pools:

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

Capacity constraints:



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

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

$$\sum x_{ij} + \sum x_{lj} \leq C_j, \quad \forall j \in J$$

Example: Pooling Problem

“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.
- This results in bilinear constraints.

Example: Pooling Problem

“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.
- This results in bilinear constraints.

- **P-formulation** (Haverly 78):
  Keep track of concentration p_{kl} of attribute k in pool l

Example: Pooling Problem

“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.
- This results in bilinear constraints.

- **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

P-formulation

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

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

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

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

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

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

Example: Pooling Problem

P-formulation

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

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

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

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

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

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

Example: Pooling Problem

Q-formulation

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

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

Example: Pooling Problem

Q-formulation

$$x_{il} = q_{il} \sum_{j \in J_l} x_{lj}, \quad \forall i \in I, l \in L_i$$
$$\sum_{i \in I_l} q_{il} = 1, \qquad \forall l \in L$$

- Attribute constraints

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

Example: Pooling Problem

Q-formulation

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

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

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

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

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

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

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:

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

Objective Function

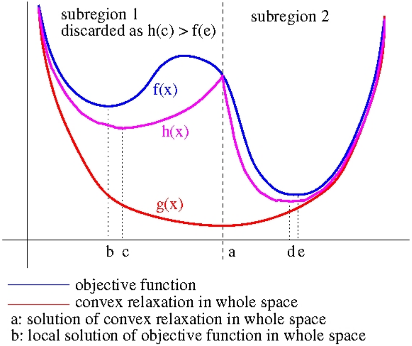
- Fixed cost for installing pipe

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

Outline

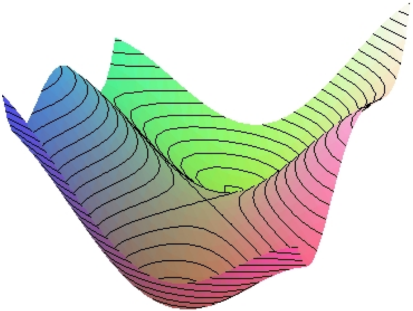
1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Global Optimization methods



Exact

- "Exact" in continuous space: ε-approximate (*find solution within pre-determined* ε *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

Outline

1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Multistart

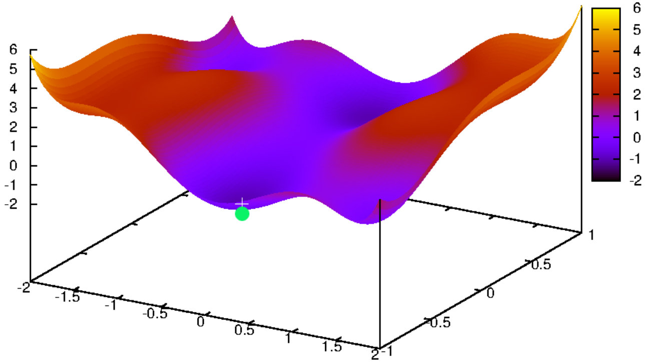
- The easiest GO method

$f^* = \infty$
$x^* = (\infty, \ldots, \infty)$
while $\neg$ termination **do**
    $x' = (\text{random}(), \ldots, \text{random}())$
    $x = \text{localSolve}(P, x')$
    if $f_P(x) < f^*$ **then**
        $f^* \leftarrow f_P(x)$
        $x^* \leftarrow x$
    end if
end while

- Termination condition: e.g. *repeat k times*

Six-hump camelback function

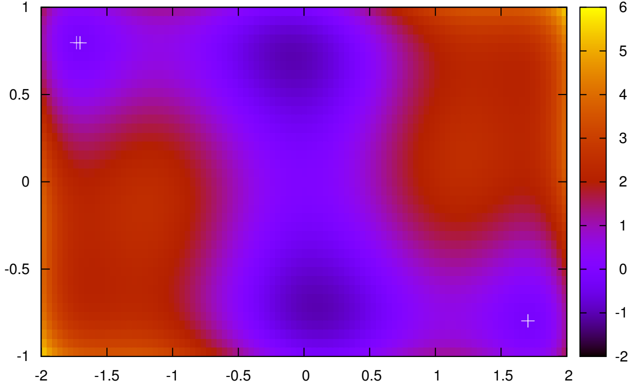
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Global optimum (COUENNE)

Six-hump camelback function

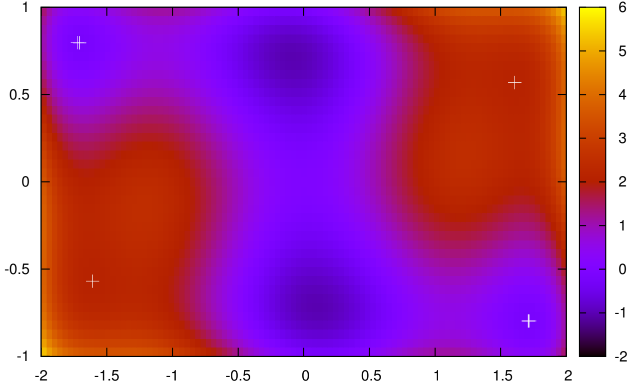
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT, $k = 5$

Six-hump camelback function

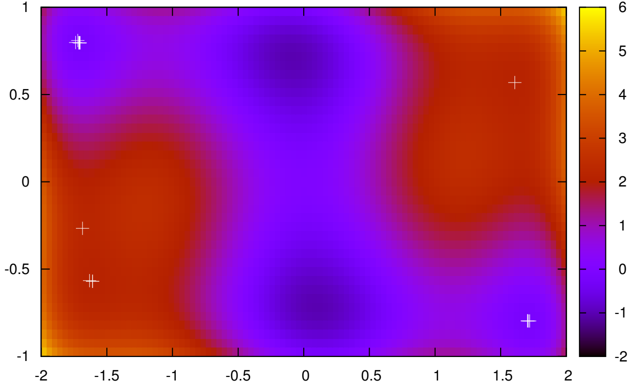
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT, $k = 10$

Six-hump camelback function

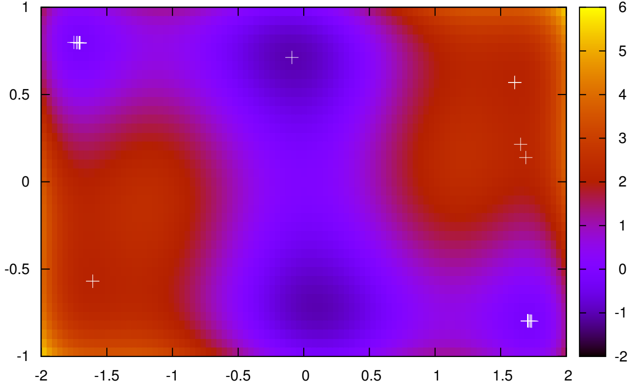
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



Multistart with IPOPT, $k = 20$

Six-hump camelback function

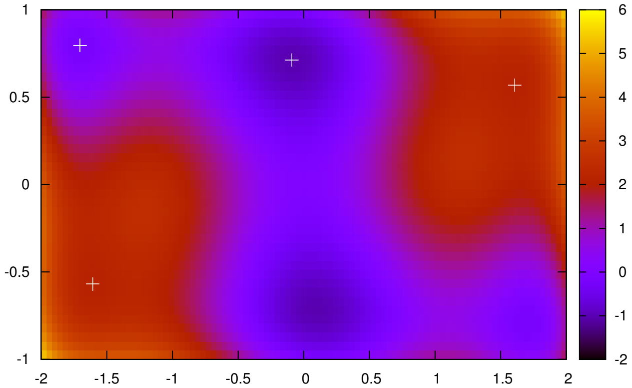
$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$



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, $k = 20$

Outline

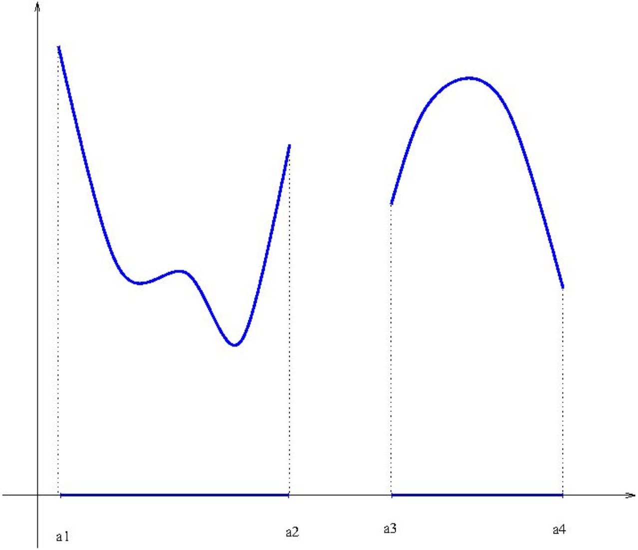
1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Spatial Branch-and-Bound

Falk and Soland (1969) "An algorithm for separable nonconvex programming problems".
35/40 years ago: first general-purpose "exact" algorithms for nonconvex MINLP.

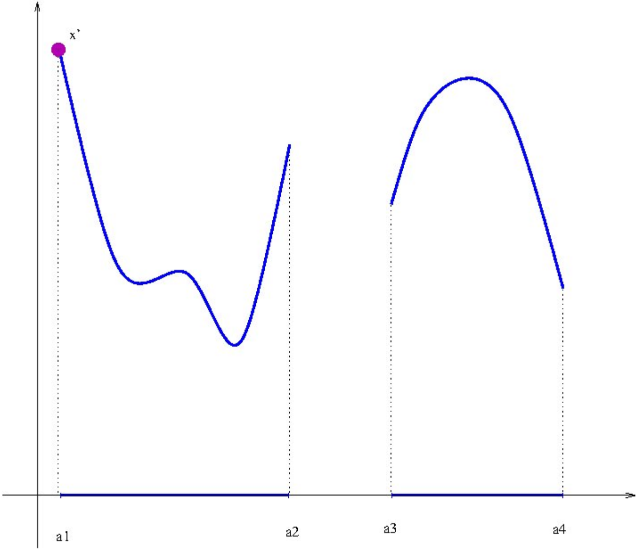
- **Tree-like search**
- Explores search space exhaustively but **implicitly**
- Builds a sequence of **decreasing upper bounds** and **increasing lower bounds** to the global optimum
- Exponential worst-case
- Only general-purpose **"exact"** algorithm for MINLP
  Since continuous vars are involved,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

Spatial B&B: Example



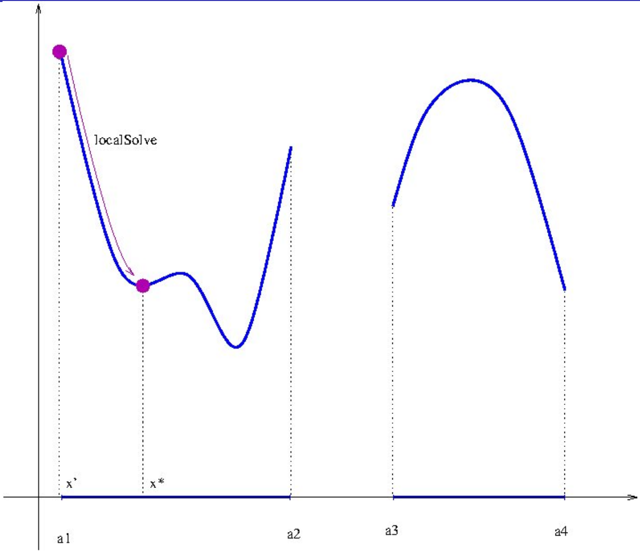
Original problem P

Spatial B&B: Example



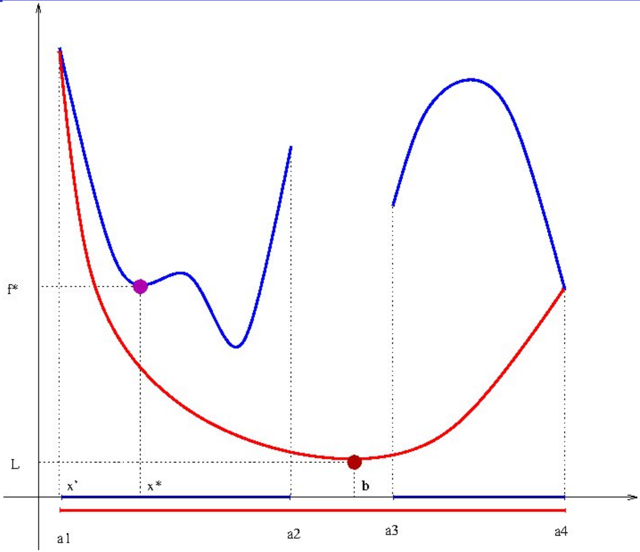
Starting point x'

Spatial B&B: Example



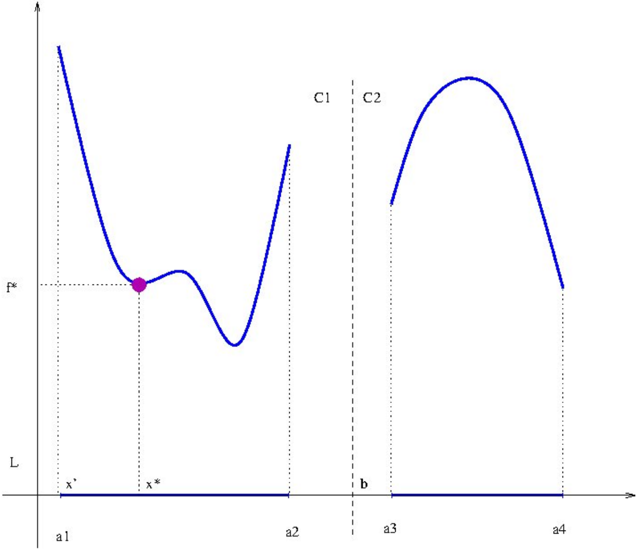
Local (upper bounding) solution x^*

Spatial B&B: Example



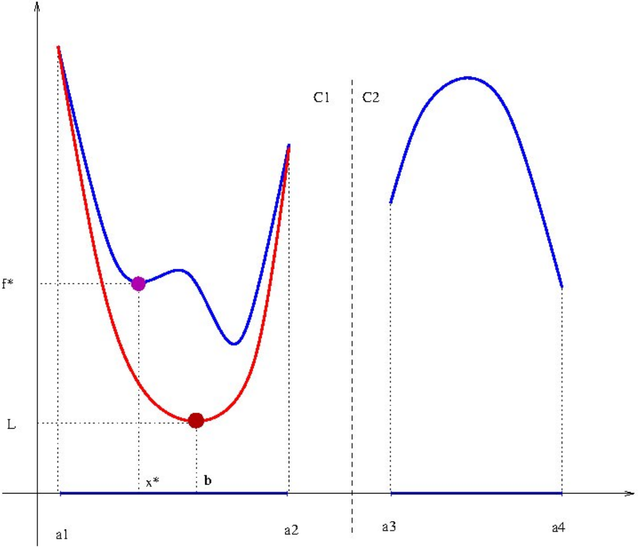
Convex relaxation (lower) bound $\bar{f}$ with $|f^* - \bar{f}| > \varepsilon$

Spatial B&B: Example



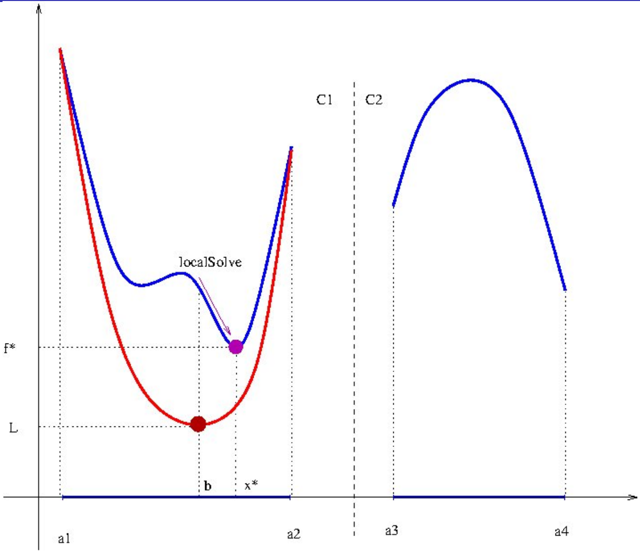
Branch at $x = \bar{x}$ into C_1, C_2

Spatial B&B: Example



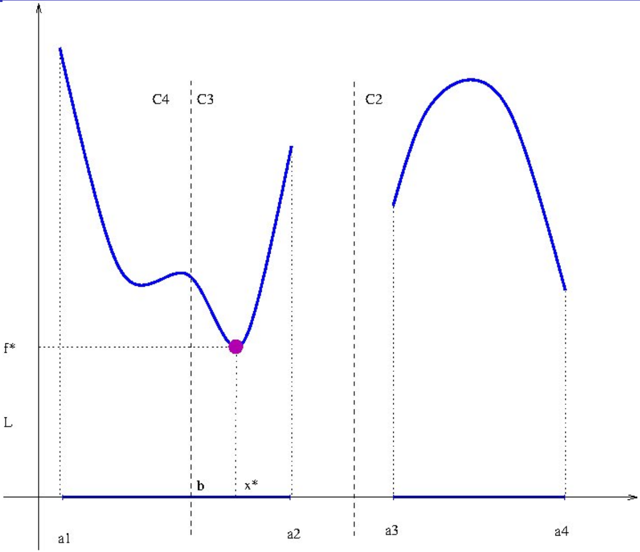
Convex relaxation on C_1: lower bounding solution $\bar{x}$

Spatial B&B: Example



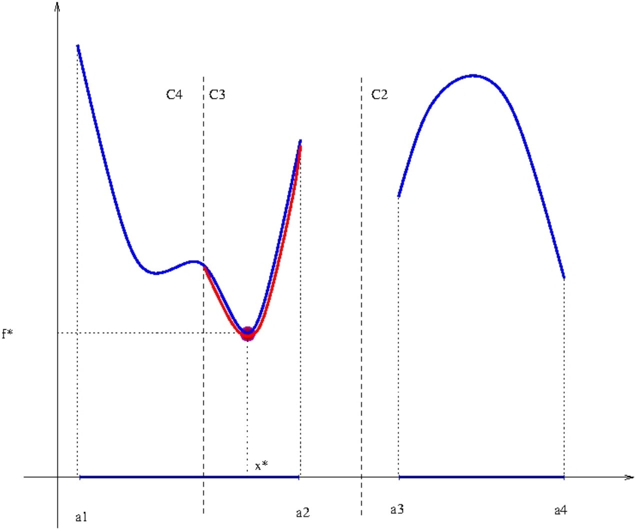
localSolve*. from $\bar{x}$: new upper bounding solution x^**

Spatial B&B: Example



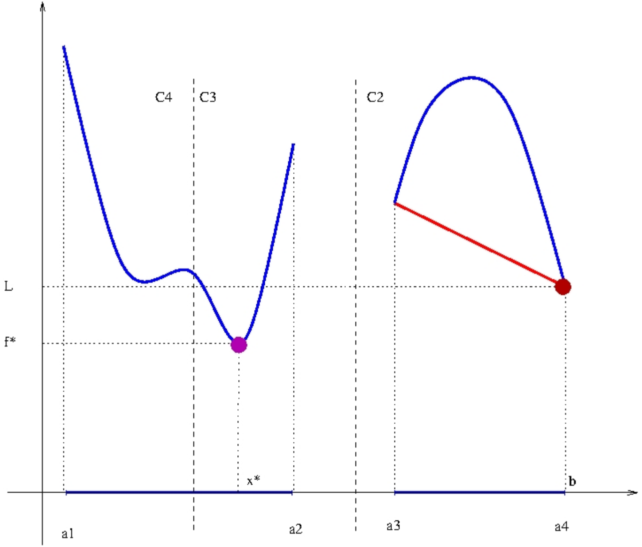
$$|f^* - \bar{f}| > \varepsilon\text{: branch at } x = \bar{x}$$

Spatial B&B: Example



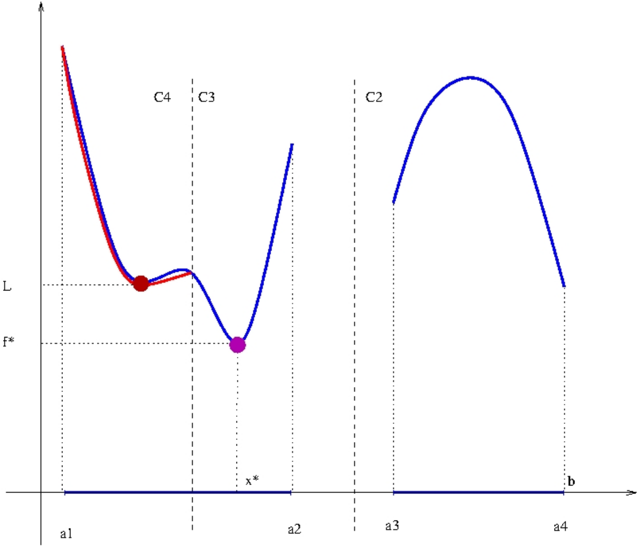
Repeat on C_3: get $\bar{x} = x^*$ and $|f^* - \bar{f}| < \varepsilon$, no more branching

Spatial B&B: Example



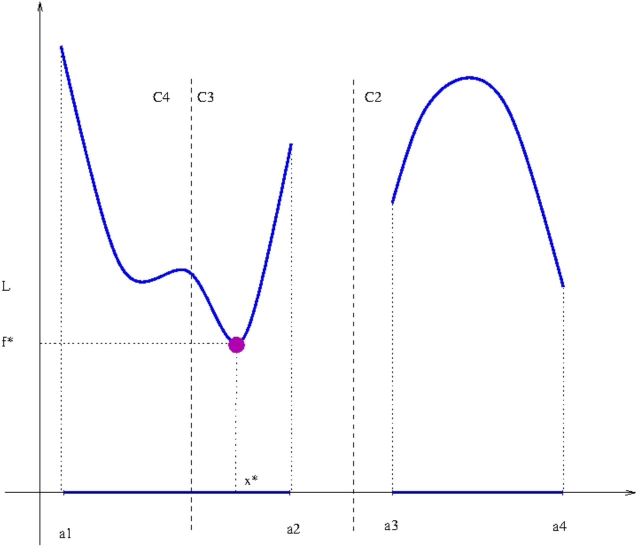
Repeat on C_2: $\bar{f} > f^*$ (can't improve x^* in C_2)

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 $\forall h, k$.

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 $\forall h, k$.

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

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 $\forall h, k$.

- 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**).

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 $\forall h, k$.

- 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.

Outline

Spatial B&B: exact reformulation to standard form

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

$$
\begin{aligned}
\min c^{\mathsf{T}}(x, w) & & \\
A(x, w) &\leq b & \\
w_{ij} &= x_i \bigotimes x_j & \text{for suitable } i, j \\
x &\in X & \\
w &\in W &
\end{aligned}
$$

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

Outline

1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Spatial B&B: convexification

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

$$\begin{aligned} w_{ij} &\leq \text{overestimator}(x_i \bigotimes x_j) \\ w_{ij} &\geq \text{underestimator}(x_i \bigotimes x_j) \end{aligned}$$

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

Spatial B&B: convexification

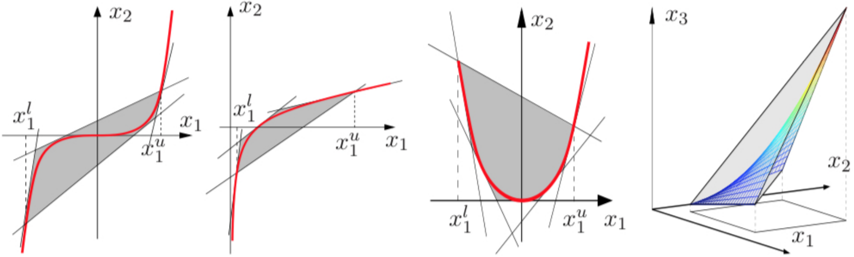
Relax $w_{ij} = x_i \bigotimes x_j$ $\forall$ suitable i, j where $\bigotimes \in$ {sum, product, quotient, power, exp, log, sin, cos, abs} such that:

$$\begin{aligned} w_{ij} &\leq \text{overestimator}(x_i \bigotimes x_j) \\ w_{ij} &\geq \text{underestimator}(x_i \bigotimes x_j) \end{aligned}$$

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



(a) $x_2 = x_1^3$ (b) $x_2 = \log x_1$ (c) $x_2 = x_1^2$ (d) $x_3 = x_1 x_2$

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

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

Example: Standard Form Reformulation

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

becomes

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

Example: .mod from Couenne

```
var x1 <= 1, >= 0;
var x2 <= 1, >= 0;

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

Example: .mod from Couenne

```
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
```

Convex hull of pieces is weaker than the whole convex hull

Consider the following feasible set:

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

Convex hull of pieces is weaker than the whole convex hull

Consider the following feasible set:

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

Convex hull: $x_1 + x_2 \geq 1$

Convex hull of pieces is weaker than the whole convex hull

Consider the following feasible set:

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

Convex hull: $x_1 + x_2 \geq 1$

Convex hull of standard form

$$\begin{aligned} x_3 + x_4 &\geq 1 \\ x_3 &\leq x_1^2 \\ x_4 &\leq x_1^2 \\ x_1, x_2 &\in [0,2] \end{aligned}$$

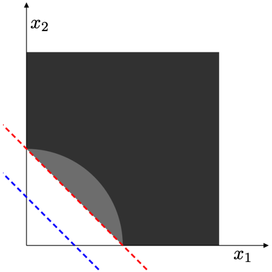


Figure: Source Belotti et al. (2013)

Outline

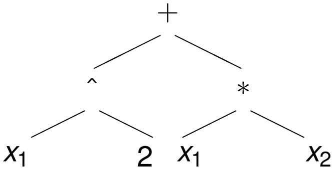
1. Recap
   - What is a MINLP?
   - Exact reformulations
   - Relaxations
2. Motivating Applications
3. Global Optimization methods
   - Multistart
   - Spatial Branch-and-Bound
     - Standard form
     - Convexification
     - Expression trees
     - Variable ranges
     - Bounds tightening
     - Reformulation Linearization Technique (RLT)

Expression trees

Representation of objective f and constraints g

Encode mathematical expressions in trees or DAGs

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

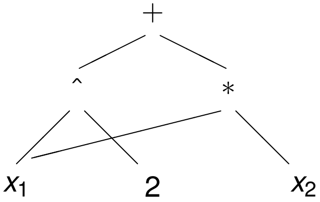


Expression trees

Representation of objective f and constraints g

Encode mathematical expressions in trees or DAGs

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



Outline

Variable ranges

- 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)

Outline

Bounds Tightening

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

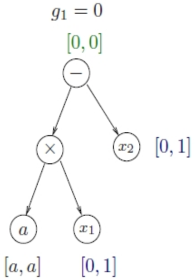
  Set $\underline{x} \leq x \leq \overline{x}$

Bounds Tightening

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

  propagation of intervals up and down constraint expression trees, with tightening at the root node

  Example: $5x_1 - x_2 = 0$.



Bounds Tightening

- In sBB we need to tighten variable bounds at each node
- Two methods:
  - Optimization Based Bounds Tightening (OBBT)
  - Feasibility Based Bounds Tightening (FBBT)
- FBBT: **propagation of intervals up and down constraint expression trees, with tightening at the root node**

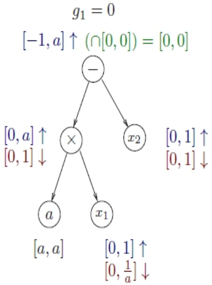
  Example: $5x_1 - x_2 = 0$.

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



Outline

RLT: Quadratic problems

- All nonlinear terms are quadratic monomials
- Aim to **reduce gap betwen 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

RLT: Quadratic problems

- For each $k \leq n$, let $w_k = (w_{k1}, \ldots, w_{kn})$

RLT: Quadratic problems

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

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

RLT: Quadratic problems

- For each $k \leq n$, let $w_k = (w_{k1}, \ldots, w_{kn})$
- 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 $z_k = (z_{k1}, \ldots, z_{kn})$

RLT: Quadratic problems

- For each $k \leq n$, let $w_k = (w_{k1}, \ldots, w_{kn})$
- 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 $z_k = (z_{k1}, \ldots, z_{kn})$
- 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

RLT: Quadratic problems

- 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

$$\begin{aligned}
\sum_{j\in J_i} x_{ij} + \sum_{l\in L_i} x_{il} &\le C_i, && \forall i \in I\\
\sum_{j\in J_l} x_{lj} &\le C_l, && \forall l \in L\\
\sum_{i\in I_j} x_{ij} + \sum_{l\in L_j} x_{lj} &\le C_j, && \forall j \in J
\end{aligned}$$

$$\begin{aligned}
x_{il} - q_{il} \sum_{j\in J_l} x_{lj} &= 0 && \forall i \in I, l \in L_i\\
\sum_{i\in I_l} q_{il} &= 1 && \forall l \in L\\
\sum_{i\in I_j} \lambda_{ki} x_{ij} + \sum_{l\in L_j} x_{lj}\Big(\sum_{i\in I_l} \lambda_{ki} q_{il}\Big) &\le \alpha_{kj} \sum_{i\in I_j\cup L_j} x_{ij}, && \forall k \in K, j \in J
\end{aligned}$$

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

PQ-formulation by Sahinidis and Tawarmalani (2005).
Like Q-formulation but with extra (redundant) constraints:

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

One of the strongest known formulation!

Citations

- 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, αBB, 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.

Advertisement...

École Polytechnique in collaboration with other universities

- **Strong formulations for Neural Networks** , when they appear as part of a mathematical optimization model
- **Optimal piecewise linear approximations** of classes of MINLPs
- **Learning for MINLPs**
- ...

Abroad

- Green Software / Data Center optimization (proposed by A. Bischi, **Università di Pisa, Italy**)
- Computer Vision from Traffic Videos / Policy Evaluation with Transfer Learning based on various sensors such as dash cam and infrastructure-based cameras / VR/AR development for Traffic Simulation and Digital Twin Development (proposed by S. Di, **Columbia University, Civil Engineering Department**)