

Fundamentals of Theory and Practice of Mixed Integer Non Linear Programming

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LIX, CNRS & École Polytechnique

STOR-i masterclass - 21 February 2019

http://www.lix.polytechnique.fr/~dambrosio/teaching/STOR-i/stor-i_2019.php

General Information

Webpage: [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)

- Lecture 1: 09:00-12:00, Thursday 21st February: **introduction, applications, methods for convex MINLPs**
- Lecture 2: 15:30-17:30, Thursday 21st February: **methods for nonconvex MINLPs**
- Lecture 3: 09:00-11:00, Friday 22nd February: **practical session**

Outline

- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Complexity
- 4 Reformulations and Relaxations
- 5 What is a convex MINLP?
- 6 Convex MINLP Algorithms
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 7 Convex functions and properties
- 8 Practical Tools

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Subset selection in Linear Regression

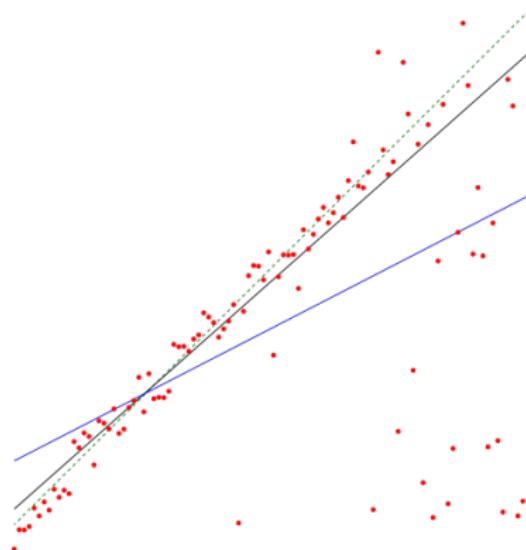
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$$\min_{\beta} \sum_i (y_i - \sum_j x_{ij} \beta_j)^2$$
$$|\text{supp}(\beta)| \leq K$$

D. Bertsimas, R. Shioda. Algorithm for cardinality-constrained quadratic optimization, **Computational Optimization and Applications**, 43 (1), pp. 1–22, 2009.

Subset selection in Linear Regression

$$\begin{aligned} \min_{\beta, z} \sum_i (y_i - \sum_j x_{ij} \beta_j)^2 \\ \sum_{j \leq d} z_j \leq K \\ \underline{\beta}_j z_j \leq \beta_j \leq \bar{\beta}_j z_j \quad \forall j \leq d \\ z_j \in \{0, 1\} \quad \forall j \leq d \end{aligned}$$

D. Bertsimas, R. Shioda. Algorithm for cardinality-constrained quadratic optimization, **Computational Optimization and Applications**, 43 (1), pp. 1–22, 2009.

Robust Portfolio Selection

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$$\begin{aligned}\min x^\top \bar{\Sigma} x \\ \bar{\mu}^\top x &\geq R \\ \mathbf{e}^\top x &= 1 \\ x &\geq 0\end{aligned}$$

where $\bar{\Sigma} \in \mathbb{R}^{n \times n}$ is the covariance return matrix, $R > 0$ is the minimum portfolio return, $\mathbf{e} \in \mathbb{R}^n$ is the all-one vector.

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H. Markowitz, Portfolio Selection, **The Journal of Finance**, 7 (1), pp. 77–91, 1952.

L. Mencarelli, C. D'Ambrosio. Complex Portfolio Selection via Convex Mixed-Integer Quadratic Programming: A Survey, **International Transactions in Operational Research** 26, pp. 389–414, 2019.

Support vector machines with the ramp loss

Support vector machines with the ramp loss

Ω set of objects, $(x_i, y_i) \forall i \in \Omega$ where $x_i \in X \subseteq \mathbb{R}^d$ and $y_i \in \{-1, +1\}$.

Support vector machines with the ramp loss

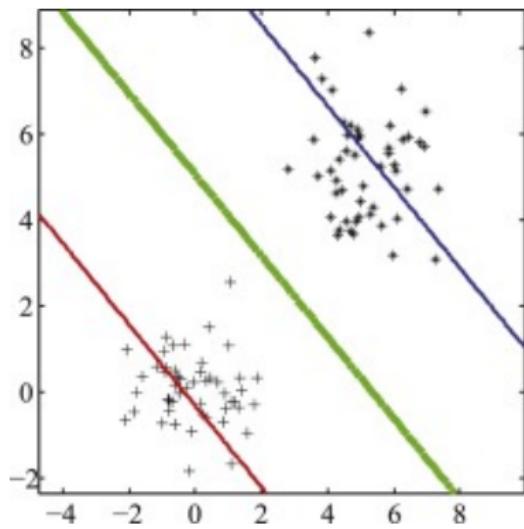
Ω set of objects, $(x_i, y_i) \forall i \in \Omega$ where $x_i \in X \subseteq \mathbb{R}^d$ and $y_i \in \{-1, +1\}$.
Aim: classify new objects by means of a hyperplane $\omega^\top x + b = 0$.

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- Penalize objects outside the margin: cost = 2
- Penalize objects within the margin ($\omega^\top x + b \in [-1, +1]$): cost in $[0, 2]$



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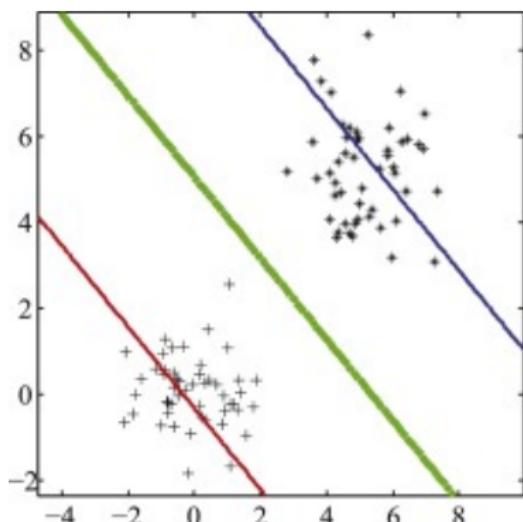
Aim: classify new objects by means of a hyperplane $\omega^\top x + b = 0$.

How to find ω and b ? Solve the following optimization problem:

$$\begin{aligned} \min_{\omega, b, \xi, z} & \frac{1}{2} \sum_{j=1}^d \omega_j^2 + \frac{C}{n} \left(\sum_{i=1}^n \xi_i + 2 \sum_{i=1}^n z_i \right) \\ & y_i(\omega^\top x_i + b) \geq 1 - \xi_i - Mz_i \quad \forall i = 1, \dots, n \\ & 0 \leq \xi_i \leq 2 \quad \forall i = 1, \dots, n \\ & z \in \{0, 1\}^n \\ & \omega \in \mathbb{R}^d \\ & b \in \mathbb{R} \end{aligned}$$

where ξ is the vector of deviation/penalty variables, z are binary variables identifying misclassification, and C is the tradeoff parameter.
If $z_i = 1$ object i is misclassified out of the margin.

Support vector machines with the ramp loss



D. Liu, Y. Shi, Y. Tian, X. Huang. Ramp loss least squares support vector machine.

Journal of Computational Science, 14, pp. 61–68, 2016.

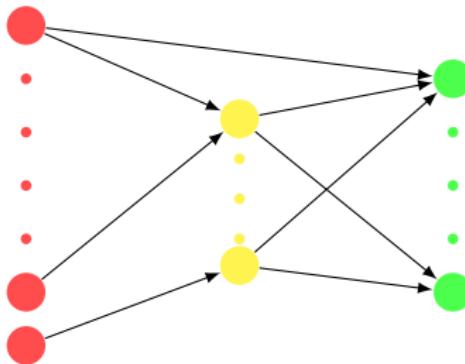
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Computational Optimization and Applications: 65(3), pp. 545–566, 2016.

Pooling Problem

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
 $\alpha_{kj}, k \in K, j \in J$

Pooling Problem: Motivation

- refinery processes in the **petroleum industry**

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- 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
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Mathematical Programming

(MINLP)

$$\min f(x, y)$$

$$g_i(x, y) \leq 0 \quad \forall i = 1, \dots, m$$

$$x \in X$$

$$y \in Y$$

where $f(x, y) : \mathbb{R}^n \rightarrow \mathbb{R}$, $g_i(x, y) : \mathbb{R}^n \rightarrow \mathbb{R} \quad \forall i = 1, \dots, m$, $X \subseteq \mathbb{R}^{n_1}$
 $Y \subseteq \mathbb{N}^{n_2}$ and $n = n_1 + n_2$.

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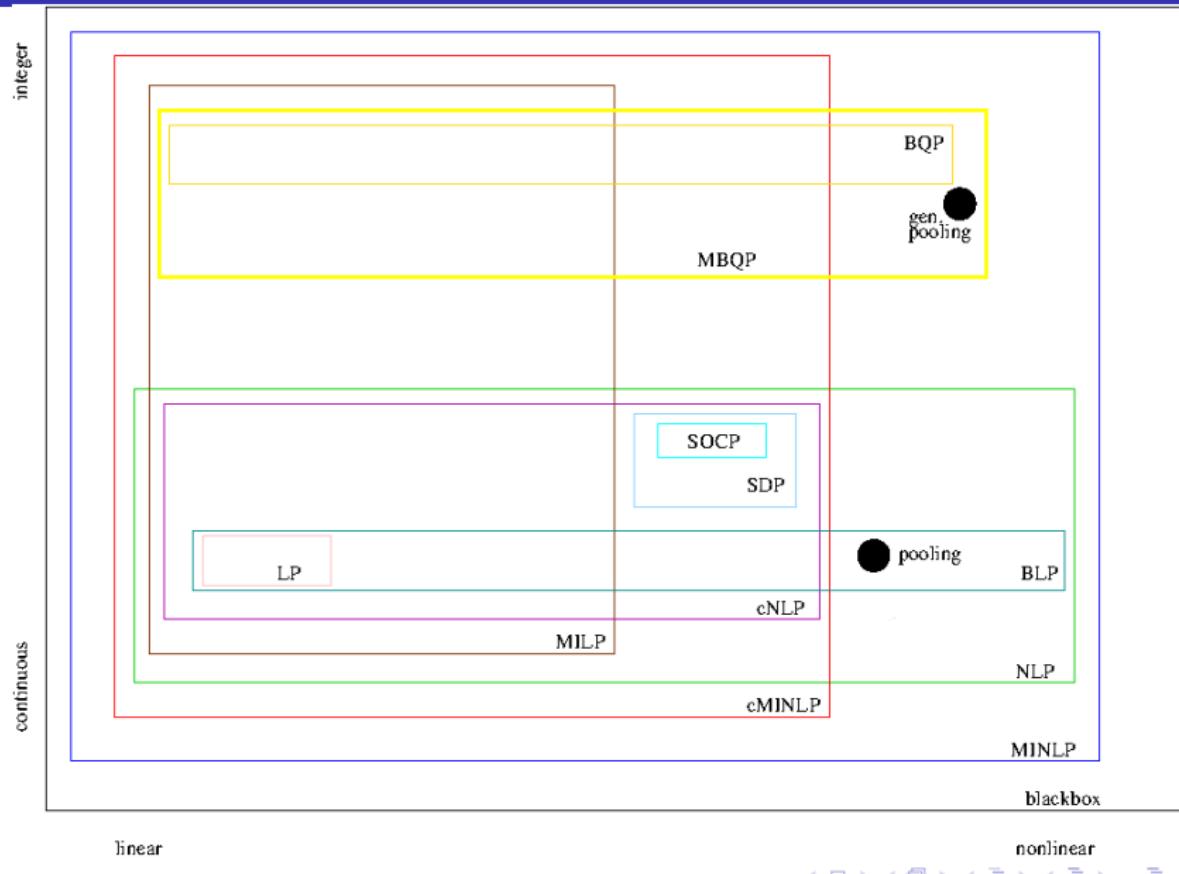
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 $Y \subseteq \mathbb{N}^{n_2}$ and $n = n_1 + n_2$.

Hypothesis: f and g are twice continuously differentiable functions.

Main optimization problem classes



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Theorem [Jeroslow, 1973]

The problem of minimizing a linear form over quadratic constraints in integer variables is not computable by a recursive function.

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Theorem [De Loera et al., 2006]

The problem of minimizing a linear function over polynomial constraints in at most 10 integer variables is not computable by a recursive function.

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Theorem [De Loera et al., 2006]

The problem of minimizing a linear function over polynomial constraints in at most 10 integer variables is not computable by a recursive function.

Solvable if we add

- $x_j^L \leq x_j \leq x_j^U \quad \forall j = 1, \dots, n_1$ and
- $y_j^L \leq y_j \leq y_j^U \quad \forall j = 1, \dots, n_2$

to (MINLP).

References

- R.G. Jeroslow, There Cannot be any Algorithm for Integer Programming with Quadratic Constraints, **Journal Operations Research**, 21 (1), pp. 221–224, 1973.
- J. A. De Loera, R. Hemmecke, M. Köppe, R. Weismantel, Integer polynomial optimization in fixed dimension, **Mathematics of Operations Research**, 31 (1), pp. 147–153, 2006.
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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 $h(w, z) : \mathbb{R}^q \rightarrow \mathbb{R}$, $p_i(w, z) : \mathbb{R}^q \rightarrow \mathbb{R} \quad \forall i = 1, \dots, r$, $W \subseteq \mathbb{R}^{q_1}$, $Z \subseteq \mathbb{N}^{q_2}$ 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.
 $\phi(w', z') = (x', y')$
- 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')

Exact reformulations

(MINLP')

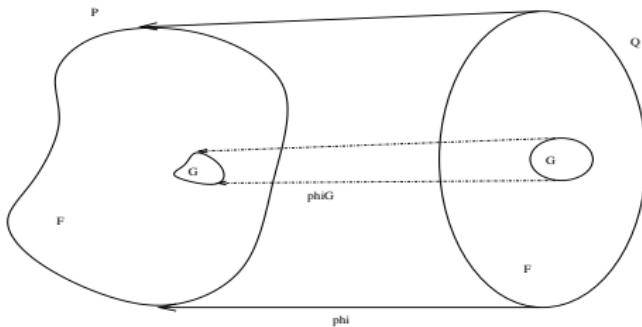
$$\min h(w, z) \quad (1)$$

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

$$w \in W \quad (3)$$

$$z \in Z \quad (4)$$

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



Exact reformulations: example 1

$$\begin{aligned} & \min y_1^2 + y_2^2 \\ & 10y_1 + 5y_2 \leq 11 \\ & y_1 \in \{0, 1\} \\ & y_2 \in \{0, 1\} \end{aligned}$$

is equivalent to

$$\begin{array}{lll} \min w_1 + w_2 & & \\ \min y_1 + y_2 & & w_1 (= y_1^2) = y_1 \\ 10y_1 + 5y_2 \leq 11 & \text{or} & w_2 (= y_2^2) = y_2 \\ y_1 \in \{0, 1\} & & 10y_1 + 5y_2 \leq 11 \\ y_2 \in \{0, 1\} & & y_1 \in \{0, 1\} \\ & & y_2 \in \{0, 1\} \end{array}$$

Exact reformulations: example 2

xy when y is binary

- If \exists bilinear term xy where $x \in [0, 1]$, $y \in \{0, 1\}$
- We can construct an **exact reformulation**:
 - Replace each term xy by an added variable w
 - Adjoin Fortet's reformulation constraints:

$$w \geq 0$$

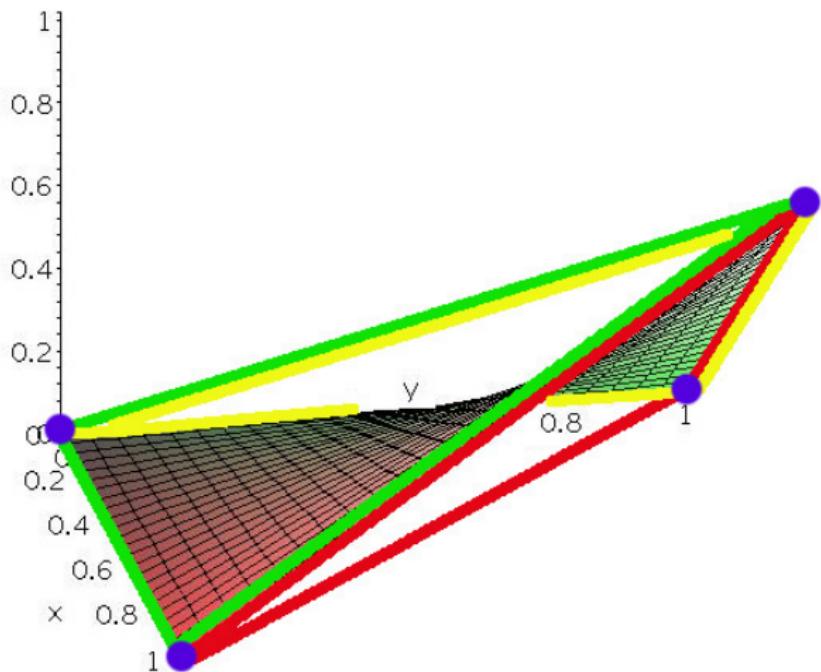
$$w \geq x + y - 1$$

$$w \leq x$$

$$w \leq y$$

- Get a MILP reformulation
- Solve reformulation using CPLEX: more effective than solving MINLP

“Proof”



“Proof”

$$w \geq 0$$

$$w \geq x + y - 1$$

$$w \leq x$$

$$w \leq y$$

$$y = 0$$

$$w \geq 0$$

$$w \geq x - 1$$

$$w \leq 0$$

$$w \leq x$$

$$y = 1$$

$$w \geq 0$$

$$w \geq x$$

$$w \leq 1$$

$$w \leq x$$

$$w = 0$$

$$w = x$$

Relaxations

(rMINLP)

$$\begin{array}{ll}\min & f(w, z) \\ \frac{g_i(w, z)}{w \in W} & \leq 0 \quad \forall i = 1, \dots, r \\ & z \in Z\end{array}$$

where $X \subseteq W \subseteq \mathbb{R}^{q_1}$, $Y \subseteq Z \subseteq \mathbb{Z}^{q_2}$, $q_1 \geq n_1$, $q_2 \geq n_2$, $f(w, z) \leq f(x, y)$
 $\forall (x, y) \subseteq (w, z)$, and

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

Examples:

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

Relaxations: example

x_1x_2 when x_1, x_2 continuous

- Get bilinear term x_1x_2 where $x_1 \in [x_1^L, x_1^U]$, $x_2 \in [x_2^L, x_2^U]$
- We can construct a **relaxation**:
 - Replace each term x_1x_2 by an added variable w
 - Adjoin following constraints:

$$\begin{aligned} w &\geq x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \\ w &\geq x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U \\ w &\leq x_1^U x_2 + x_2^L x_1 - x_1^U x_2^L \\ w &\leq x_1^L x_2 + x_2^U x_1 - x_1^L x_2^U \end{aligned}$$

- These are called **McCormick's envelopes**
- Get an LP relaxation (solvable in polynomial time)

References & Software

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What is a convex MINLP?

Convex Mixed Integer NonLinear Programming (MINLP).

$$\min f(x, y)$$

$$g(x, y) \leq 0$$

$$x \in X = \{x \mid x \in \mathbb{R}^{n_1}, Dx \leq d, x^L \leq x \leq x^U\}$$

$$y \in Y = \{y \mid y \in \mathbb{Z}^{n_2}, Ay \leq a, y^L \leq y \leq y^U\}$$

with $f(x, y) : \mathbb{R}^{n_1+n_2} \rightarrow \mathbb{R}$ and $g(x, y) : \mathbb{R}^{n_1+n_2} \rightarrow \mathbb{R}^m$ are

- * continuous

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- * continuous
- * twice differentiable

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functions.

- Local optima are also global optima .

“Basic” subproblems
we can solve “well”

NLP relaxation

$$\min f(x, y)$$

$$g(x, y) \leq 0$$

$$x \in X$$

$$y \in \{y \mid Ay \leq a\}$$

$$y_j \leq \alpha_j^k \quad j \in \{1, 2, \dots, n_2\}$$

$$y_j \geq \beta_j^k \quad j \in \{1, 2, \dots, n_2\}$$

k : current step of a Branch-and-Bound procedure;

α^k : current lower bound on y ($\alpha^k \geq y^L$);

β^k : current upper bound on y ($\beta^k \leq y^U$).

NLP restriction and Feasibility subproblem

NLP restriction for a fixed y^k :

$$\begin{aligned} & \min f(x, y^k) \\ & g(x, y^k) \leq 0 \\ & x \in X. \end{aligned}$$

NLP restriction and Feasibility subproblem

NLP restriction for a fixed y^k :

$$\begin{aligned} & \min f(x, y^k) \\ & g(x, y^k) \leq 0 \\ & x \in X. \end{aligned}$$

Feasibility subproblem for a fixed y^k :

$$\begin{aligned} & \min u \\ & g(x, y^k) \leq u \\ & x \in X \\ & u \in \mathbb{R}_+. \end{aligned}$$

MILP relaxation

$$\begin{aligned} & \min \gamma \\ f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} & \leq \gamma \quad \forall k \\ g_i(x^k, y^k) + \nabla g_i(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} & \leq 0 \quad \forall k \ \forall i \in I^k \\ x & \in X \\ y & \in Y. \end{aligned}$$

where $I^k \subseteq \{1, 2, \dots, m\}$.

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- $I^k = \{1, 2, \dots, m\}$
- $I^k = \{i \mid g_i(x^k, y^k) > 0, 1 \leq i \leq m\}$

Outline

- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Complexity
- 4 Reformulations and Relaxations
- 5 What is a convex MINLP?
- 6 Convex MINLP Algorithms
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 7 Convex functions and properties
- 8 Practical Tools

Convex MINLP Algorithms

- Branch-and-Bound (BB).

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Gupta and Ravindran, 1985. Link BB for MILPs.

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Fathoming is performed when:

- The subproblem solution is MINLP feasible (f^*).

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Fathoming is performed when:

- The subproblem solution is MINLP feasible (f^*).
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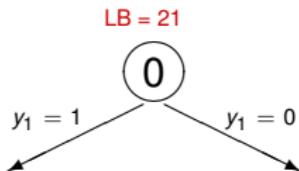
- The subproblem solution is MINLP feasible (f^*).
- The subproblem is infeasible.
- The subproblem P^k has $LB(P^k) \geq f^*$.

Branch-and-Bound (BB)

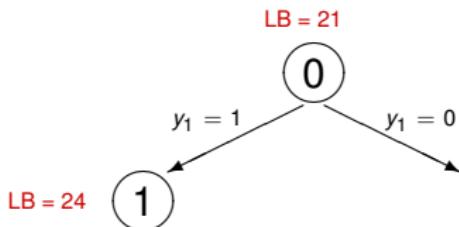
LB = 21

0

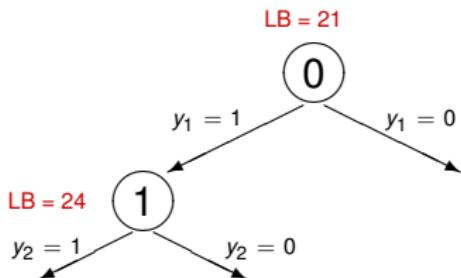
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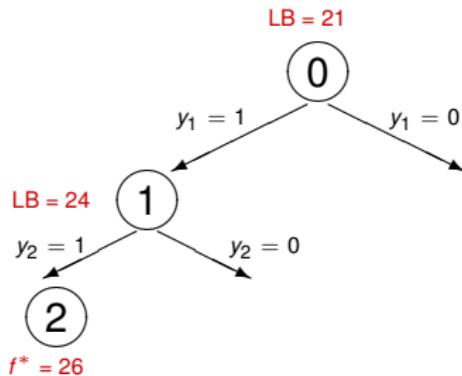
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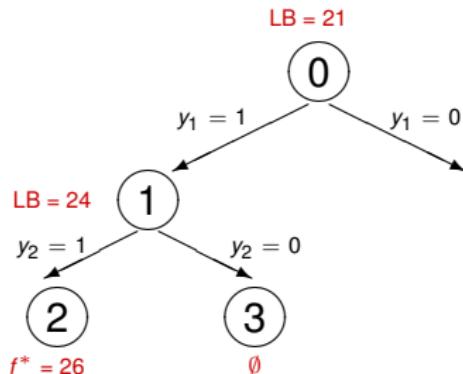
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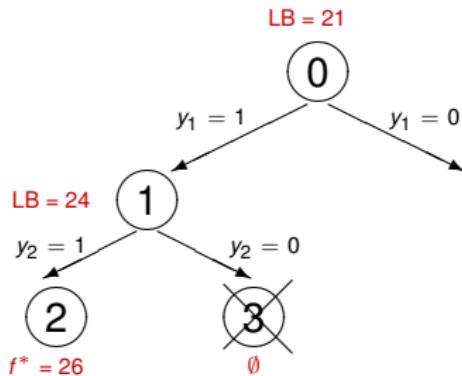
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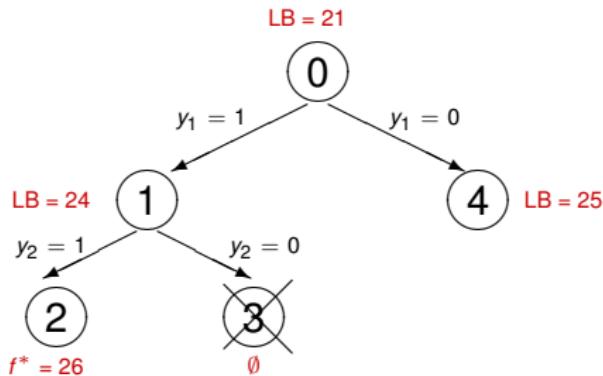
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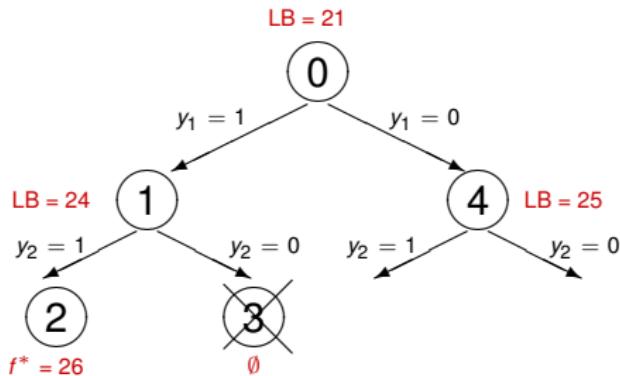
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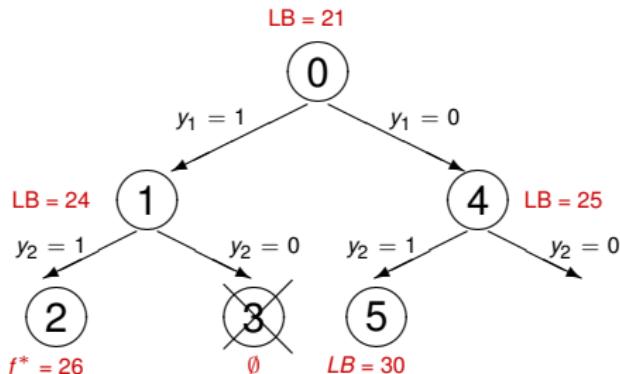
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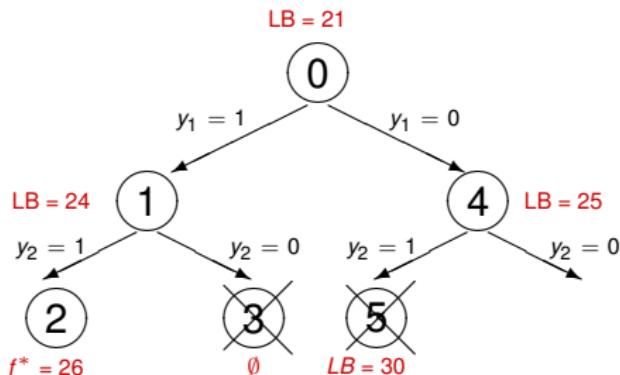
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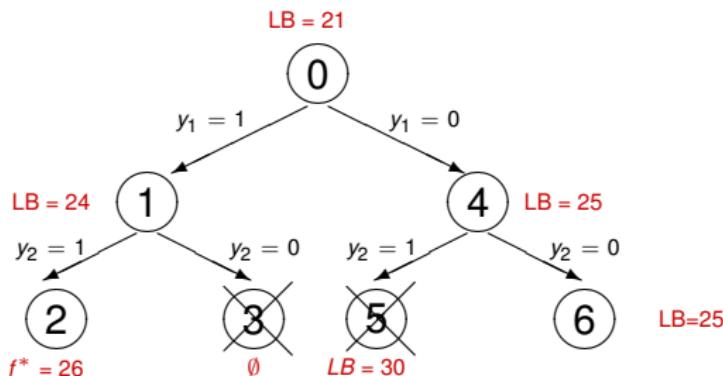
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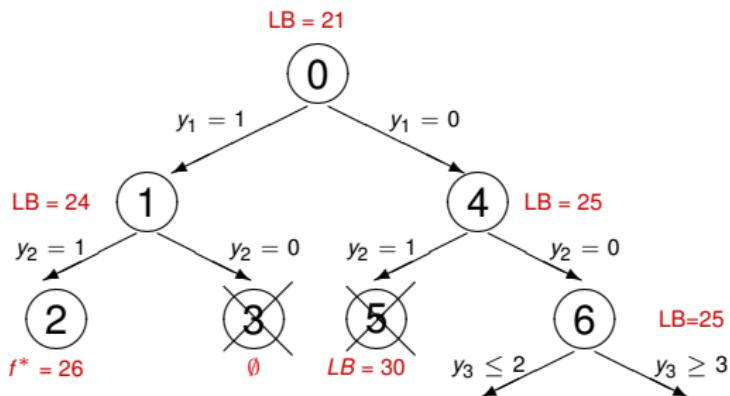
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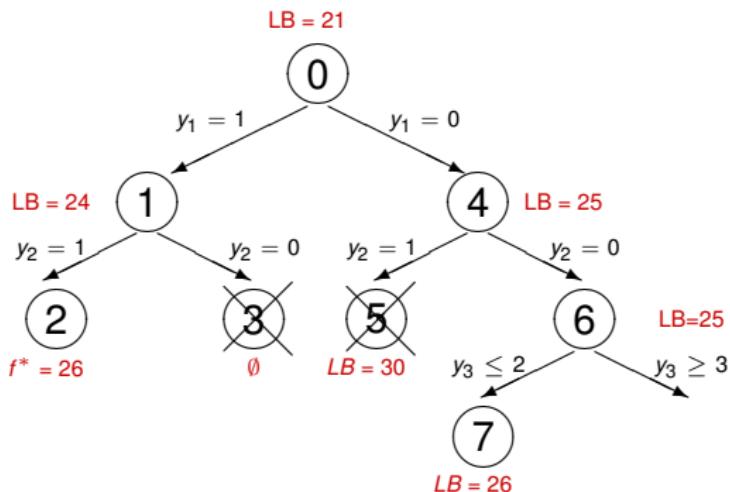
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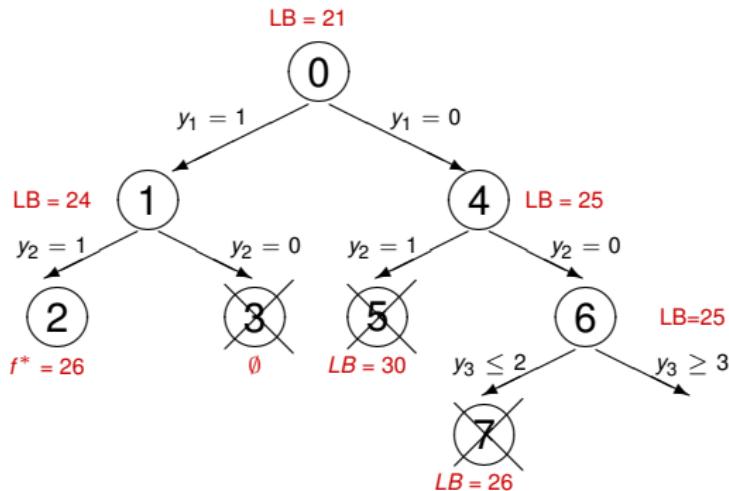
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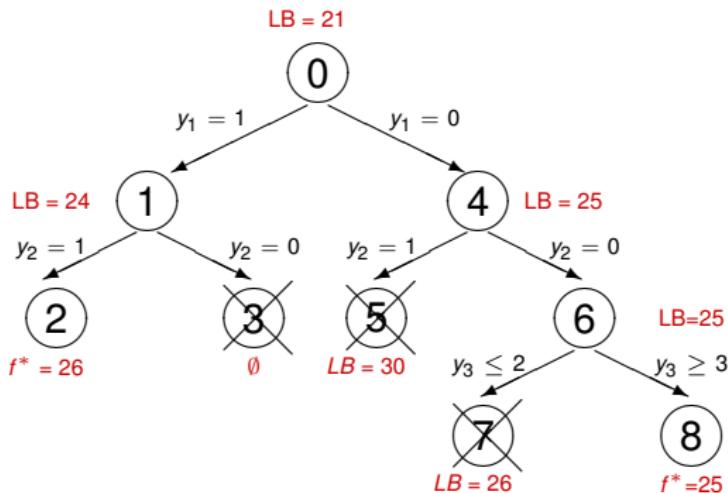
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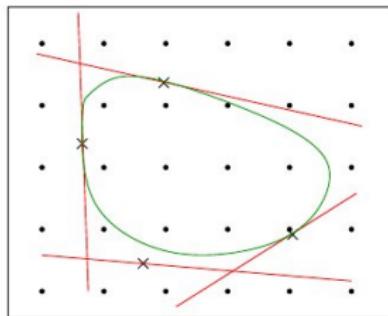


Outer-Approximation (OA)

Duran and Grossmann, 1986.

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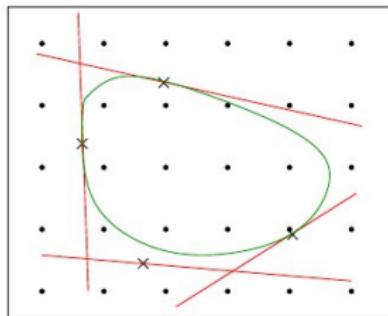
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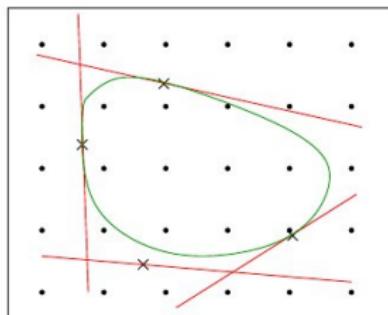


$$I^k = \{1, 2, \dots, m\} \quad \forall k = 1, \dots, K.$$

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NB. The linearization constraints of MILP relaxation are not valid for non-convex MINLPs.

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- 1: $K = 1$, define an initial MILP relaxation, $f^* = +\infty$, LB = $-\infty$.
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Proof.

(Sketch of) It can be shown that the constraints of GDB MILP relaxation are surrogate of the ones of OA MILP relaxation (see, Quesada and Grossmann, 1992). 

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Example of cut in the infeasible case:

$$\sum_{i=1}^m \lambda_i^k \left(g_i(x^k, y^k) + \nabla g_i(x^k, y^k)^T (y - y^k) \right) \leq 0 \quad \forall k \quad \forall i \in I^k$$

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More iterations needed wrt OA.

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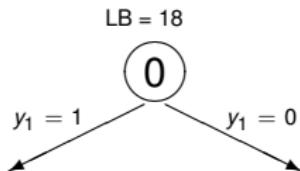
Link OA, but only 1 MILP relaxation is solved, and updated in the tree search.

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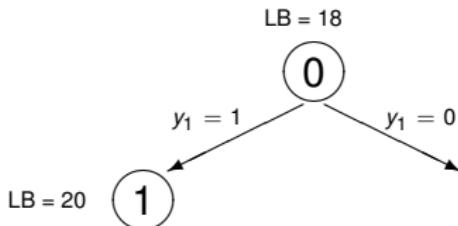
LB = 18

0

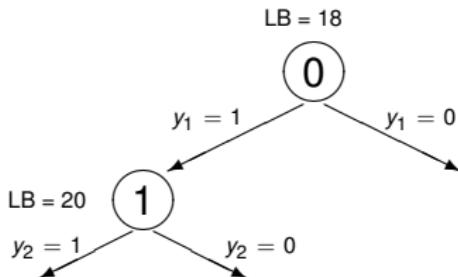
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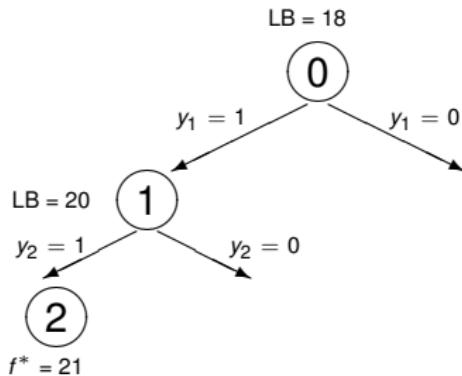
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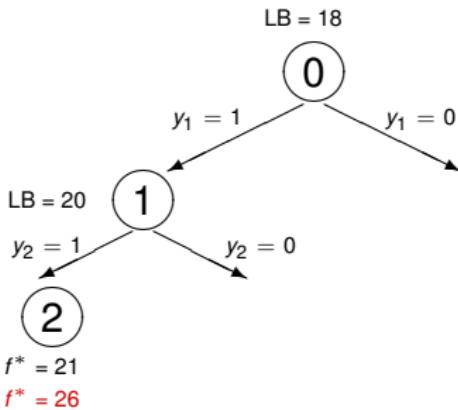
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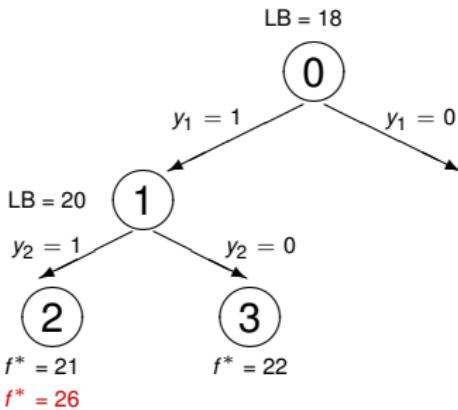
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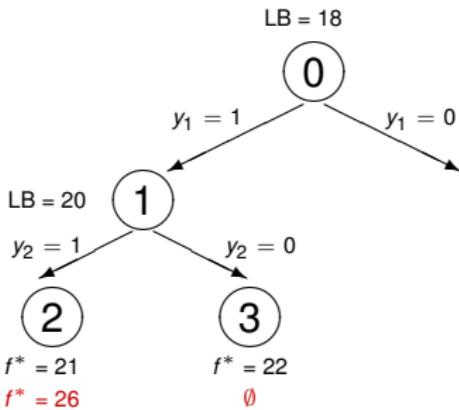
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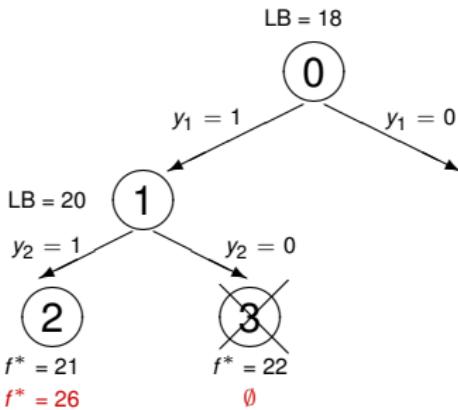
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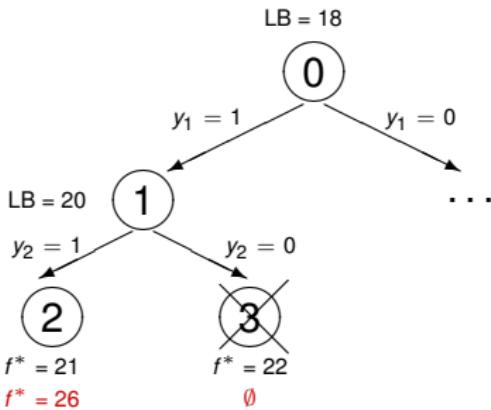
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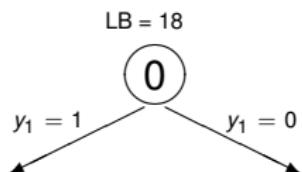
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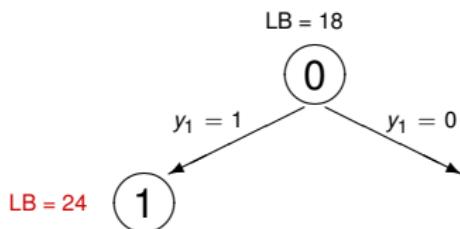
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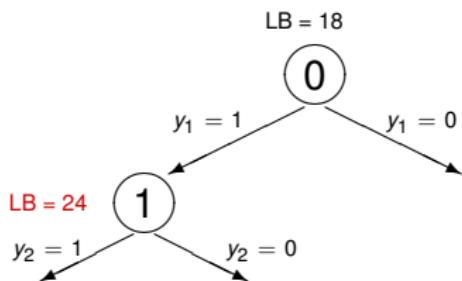
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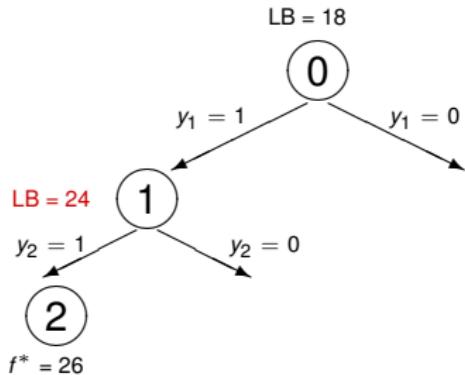
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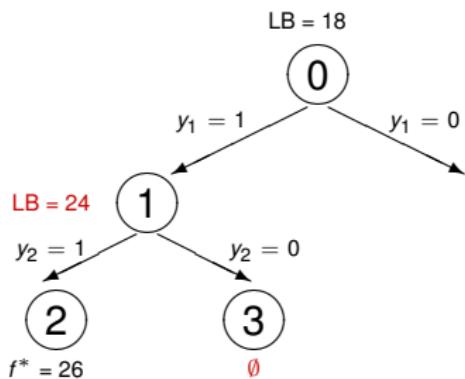
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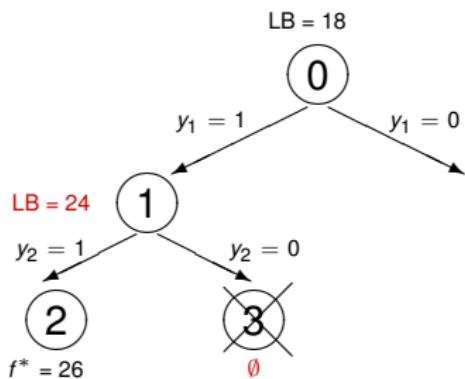
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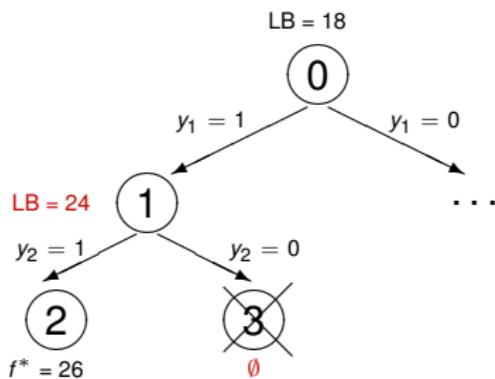
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Number of subproblems solved

	# MILP	# NLP	note
BB	0	# nodes	
OA	# iterations	# iterations	
GBD	# iterations	# iterations	1
ECP	# iterations	0	
QG	1	1 + # explored MILP solutions	
Hyb ALL10	1	1 + # explored MILP solutions	2
Hyb CMUIBM	1	[# explored MILP solutions, # nodes]	

Table: Number of MILP and NLP subproblems solved by each algorithm.

¹weaker lower bound w.r.t. OA, MILP with less constraints than the one of OA

²stronger lower bound w.r.t. QG ,MILP with more constraints than the one of QG

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Outline

- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Complexity
- 4 Reformulations and Relaxations
- 5 What is a convex MINLP?
- 6 Convex MINLP Algorithms
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 7 Convex functions and properties
- 8 Practical Tools

Reminder: Convex functions and some properties

Properties:

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$$\max\{f_1(x), f_2(x), \dots, f_m(x)\}$$
- Composition, e.g., $f_2(f_1(x))$ if f_1 convex and f_2 nondecreasing and convex or f_1 concave and f_2 nonincreasing and convex
- Minimization, e.g., $\inf_{z \in C} f(x, z)$

Outline

- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Complexity
- 4 Reformulations and Relaxations
- 5 What is a convex MINLP?
- 6 Convex MINLP Algorithms
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 7 Convex functions and properties
- 8 Practical Tools

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Modeling Languages

Modeling languages, e.g., AMPL, GAMS, JUMP.

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Example:

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param pi := 3.142;
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set VARS ordered := {1..N};
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param U {j in VARS};
param a {j in VARS};
param b {j in VARS};
param c {j in VARS};
param d {j in VARS};
param w{VARS};
param C;
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NEOS: [http://www.neos-server.org/neos/.](http://www.neos-server.org/neos/)

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The screenshot shows a Mozilla Firefox window with the title "Optimization Tree - NEOS - Mozilla Firefox". The address bar contains the URL http://www.neos-guide.org/NEOS/index.php/Optimization_Tree. The page itself is titled "Optimization Tree" and features a sidebar with navigation links for NEOS Wiki, NEOS Server, Optimization Tree, Software Guide, etc. The main content area is divided into several sections: "Continuous Optimization", "Discrete and Integer Optimization", "Optimization Under Uncertainty", "Complementarity Constraints and Variational Inequalities", "Systems of Equations and Inequalities", and "Multiobjective Programming". Each section lists various sub-topics. At the bottom of the page, there is footer information including copyright notices for the University of Wisconsin-Madison and Morgridge Institute for Discovery, along with links to "About NEOS" and "Terms of Use".

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- QPLIB: 367 instances

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- When modeling a problem, do not forget to define simple bounds on each variable
- Exactly reformulate nonlinear term, if possible
- Several tailored methods for convex MINLPs (not exact for nonconvex MINLPs)
- Identifying convexity is, in general, very difficult

In fact the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.

R. T. Rockafellar. Lagrange multipliers and optimality. SIAM Review, 35:183–238, 1993.