

Mixed Integer Non Linear Optimization: Methods and Applications

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Mixed Integer Nonlinear Programming

Claudia D'Ambrosio
dambrosio@lix.polytechnique.fr



- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Reformulations and Relaxations
- 4 Convex MINLP
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 5 Convex functions and properties
- 6 Practical Tools
- 7 Tomorrow: nonconvex MINLPs

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Robust Portfolio Selection

Robust Portfolio Selection

- n possibly risky assets
- mean return vector $\bar{\mu} \in \mathbb{R}^n$
- Variables: $x \in \mathbb{R}_+^n$: fraction of the portfolio value invested in each of the n assets

$$\min x^T \bar{\Sigma} x$$

$$\bar{\mu}^T x \geq R$$

$$\mathbf{e}^T x = 1$$

$$x \geq 0$$

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.

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

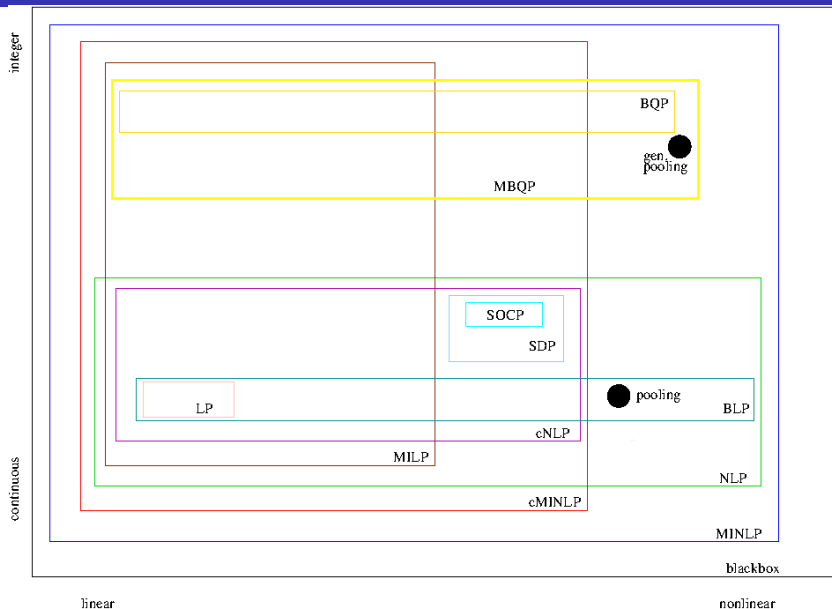
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Hypothesis: f and g are twice continuously differentiable functions.

Main optimization problem classes



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

Exact reformulations

(MINLP')

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

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

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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')

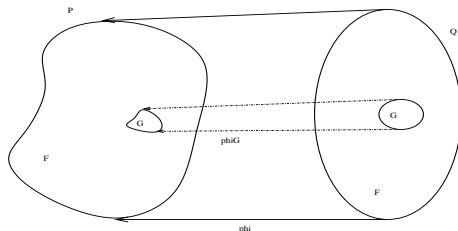
$$\min h(w, z) \quad (1)$$

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

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

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

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

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

is equivalent to

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

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:

$$w \geq 0$$

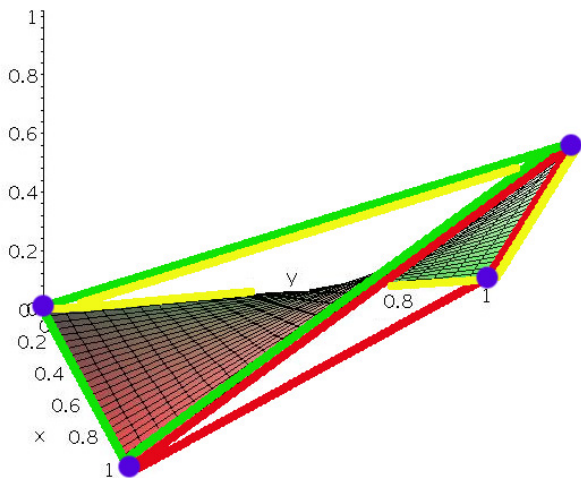
$$w \geq x + y - 1$$

$$w \leq x$$

$$w \leq y$$

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

“Proof”



“Proof”

$$w \geq 0$$

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

$$w \leq x$$

$$w \leq y$$

$$y = 0$$

$$w \geq 0$$

$$w \geq x - 1$$

$$w \leq 0$$

$$w \leq x$$

$$w = 0$$

$$y = 1$$

$$w \geq 0$$

$$w \geq x$$

$$w \leq 1$$

$$w \leq x$$

$$w = x$$

Exact reformulations: example 3

(MINLP)

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

Exact reformulations: example 3

(MINLP)

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

(MINLP')

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

Exact reformulations: example 3

(MINLP)

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

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

$$x \in X$$

$$y \in Y$$

(MINLP')

$$\min \gamma$$

$$\gamma \geq f(x, y)$$

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Exact reformulations: example 3

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- The optimal solutions of (MINLP) are **not necessarily on the boundaries** of the convex hull of the feasible set

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- The optimal solutions of (MINLP) are **not necessarily on the boundaries** of the convex hull of the feasible set
- The optimal solutions of (MINLP') are **on the boundaries** of the convex hull of the feasible set

(MINLP') interesting reformulation for cutting plane methods

(otherwise, cannot “separate” from the feasible set)

Relaxations

(rMINLP)

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

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

Relaxations: example

$x_1 x_2$ when x_1, x_2 continuous

- Get bilinear term $x_1 x_2$ 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 $x_1 x_2$ 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)

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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** .

- Branch-and-Bound (BB).

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NLP relaxation

$$\begin{aligned} \min & f(x, y) \\ & g(x, y) \leq 0 \\ & x \in X \\ & y \in \{y \mid Ay \leq a\} \\ & y_j \leq \alpha_j^k & j \in \{1, 2, \dots, n_2\} \\ & y_j \geq \beta_j^k & j \in \{1, 2, \dots, n_2\} \end{aligned}$$

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 ($\beta^k \leq y^U$).

Branch-and-Bound (BB)

Gupta and Ravindran, 1985. Link BB for MILPs.

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- 2: **while** $\Pi \neq \emptyset$ **do**

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- 4: Solve P obtaining $(\bar{x}, \bar{y})$.

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- 6: **continue**
- 7: **end if**
- 8: **if** $\bar{y} \in \mathbb{Z}^{n_2}$ **then**
- 9: $f^* = f(\bar{x}, \bar{y})$, $(x^*, y^*) = (\bar{x}, \bar{y})$.

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- 10: Update Π potentially fathoming subproblems.

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- 11: **else**
- 12: Take a fractional value $\bar{y}_j$ and obtain two subproblems $P^1 = P$ with $\alpha_j^1 = \lfloor \bar{y}_j \rfloor$ and $P^2 = P$ with $\beta_j^2 = \lfloor \bar{y}_j \rfloor + 1$.

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- 13: $LB(P^1) = LB(P^2) = f(\bar{x}, \bar{y})$.
- 14: $\Pi = \Pi \cup \{P^1, P^2\}$.

Branch-and-Bound (BB)

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```
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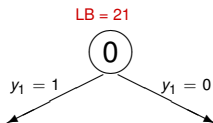
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- The subproblem P^k has $LB(P^k) \geq f^*$.

Branch-and-Bound (BB)

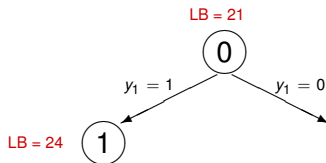
LB = 21

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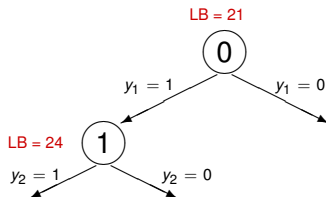
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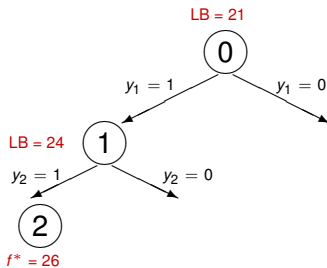
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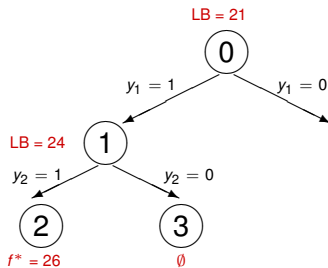
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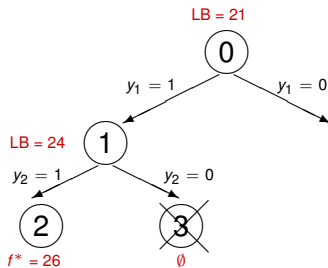
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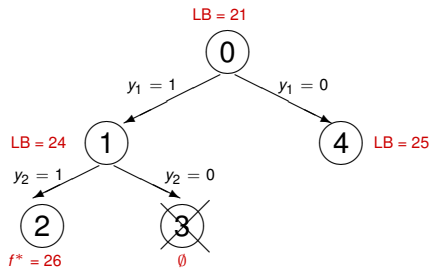
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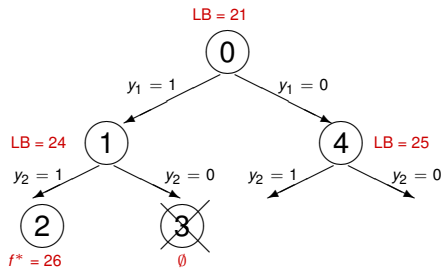
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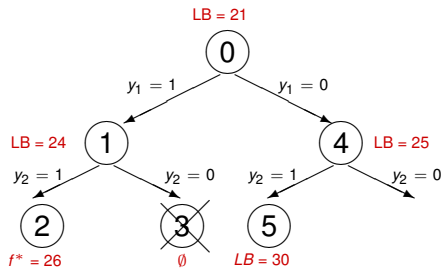
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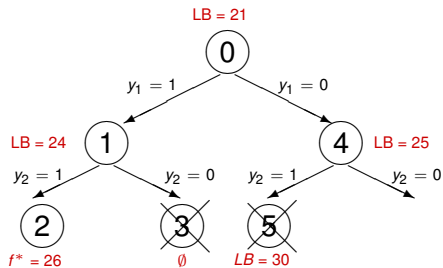
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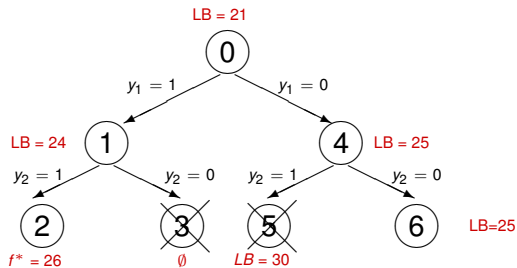
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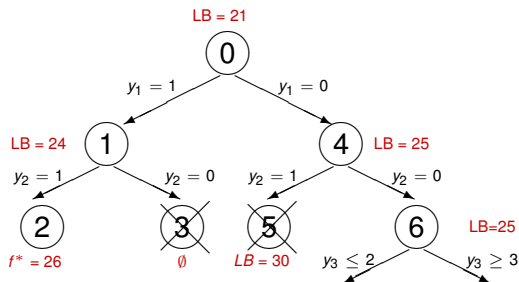
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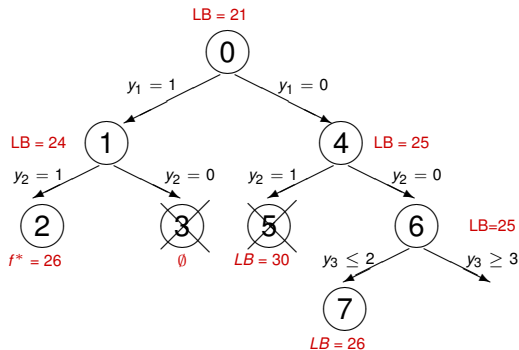
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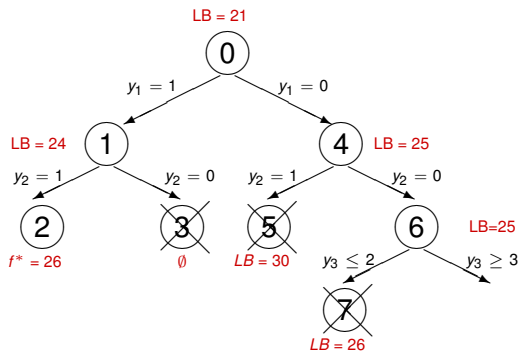
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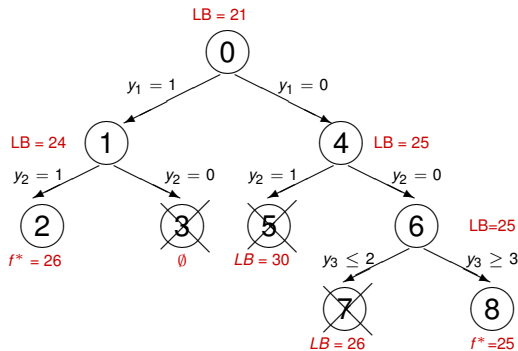
Branch-and-Bound (BB)



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Branch-and-Bound (BB)



Proposition

If the functions f and g are convex and twice continuously differentiable, X and Y are bounded, it follows that branch-and-bound terminates at an optimal solution after searching a finite number of nodes (or that the instance is infeasible).

Proof.

- Every NLP node can be solved to global optimality
- As X and Y are bounded, the B&B tree is finite
- Thus, similar proof for MILP B&B (see Th. 24.1 of Schrijver (1986)).



Outline

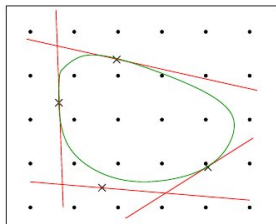
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Outer-Approximation (OA)

Duran and Grossmann, 1986.

Outer-Approximation (OA)

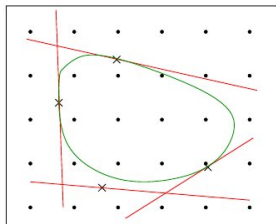
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$$\begin{aligned} \min \gamma \\ f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} &\leq \gamma \quad \forall k \\ g_i(x^k, y^k) + \nabla g_i(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} &\leq 0 \quad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

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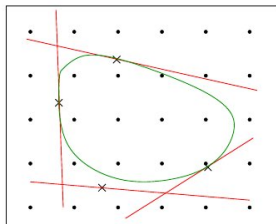


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NB. The linearization constraints of MILP relaxation are not valid for non-convex MINLPs.

Outer-Approximation (OA)

MILP relaxation

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NLP restriction and Feasibility subproblem

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Feasibility subproblem for a fixed y^k :

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

Worst-case complexity of outer approximation

Hijazi et al. (2013)

$$\sum_{i=1}^n \left(x_i - \frac{1}{2} \right)^2 \leq \frac{n-1}{4}$$
$$x \in \{0, 1\}^n$$

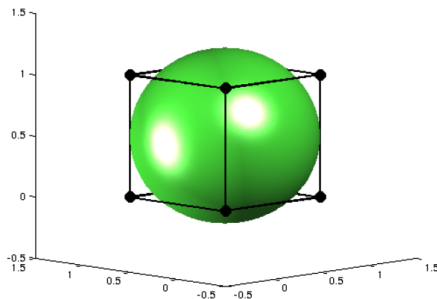


Figure: Source Belotti et al. (2013)

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Proposition

Given the same set of K subproblems, the LB provided by the MILP relaxation of OA is $\geq$ of the one provided by the MILP relaxation of GDB.

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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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- 5: **return** (x^K, y^K) (optimal solution).
- 6: **else**
- 7: Generate (some) new linearization constraints from (x^K, y^K)
and update MILP relaxation.

Extended Cutting Plane (ECP)

Westerlund and Pettersson, 1995.

- 1: $K = 1$, obtain an initial MILP relaxation.
 - 2: **while do**
 - 3: Solve the MILP relaxation obtaining (x^K, y^K) .
 - 4: **if** no constraint is violated by (x^K, y^K) **then**
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 - 8: **end if**
 - 9: $K = K + 1$.
 - 10: **end while**
- More iterations needed wrt OA.

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

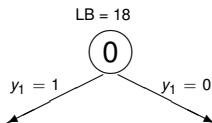
Finite convergence as for B&B.

LP/NLP-based Branch-and-Bound (QG)

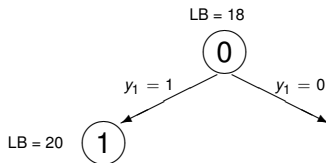
LB = 18

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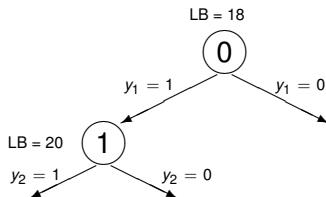
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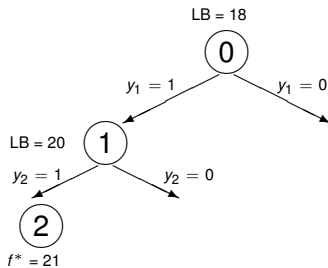
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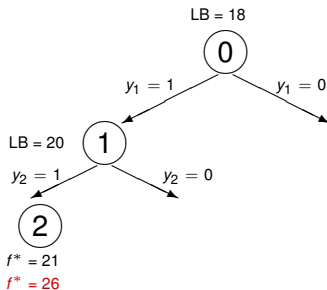
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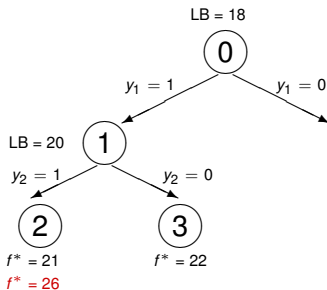
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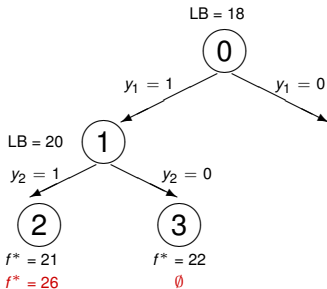
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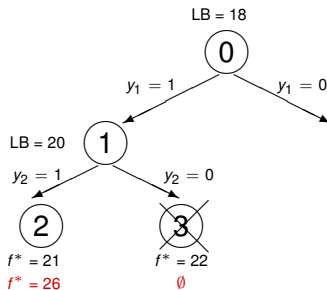
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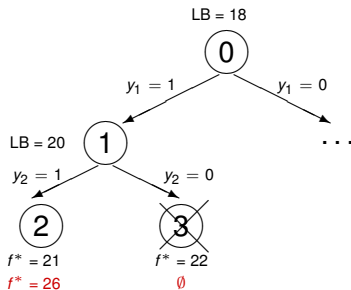
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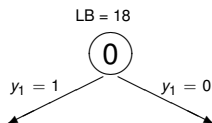
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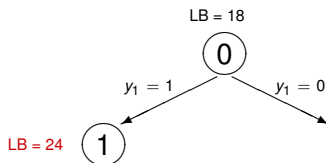
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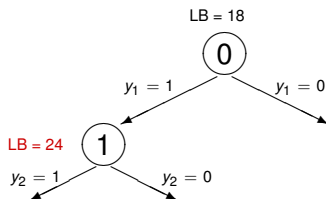
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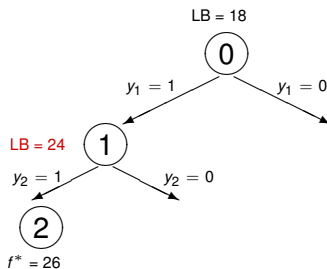
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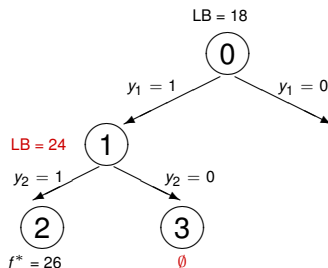
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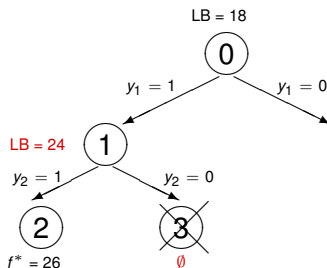
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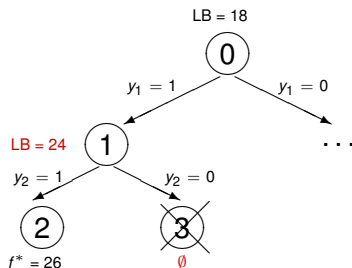
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Number of subproblems solved

	# MILP	# NLP	note
BB	0	# nodes	1
OA	# iterations	# iterations	
GBD	# iterations	# iterations	
ECP	# iterations	0	
QG	1	1 + # explored MILP solutions	2
Hyb ALL10	1	1 + # explored MILP solutions	
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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Reminder: Convex functions and some properties

Properties:

- $\forall x_1, x_2 \in X, \forall t \in [0, 1] : \quad f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2).$

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Modeling Languages

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

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Example:

```
param pi := 3.142;  
param N;  
set VARS ordered := {1..N};  
param Umax default 100;  
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/>.

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Optimization Tree - NEOS - Mozilla Firefox

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Optimization Tree

Introduction to Optimization
Taxonomy of Optimization Tree

Continuous Optimization

- Unconstrained Optimization
- Bound Constrained Optimization
- Derivative-Free Optimization
- Global Optimization
- Linear Programming
- Network Flow Problems
- Nondifferentiable Optimization
- Nonlinear Programming
- Optimization of Dynamic Systems
- Quadratic Constrained Quadratic Programming
- Quadratic Programming
- Second Order Cone Programming
- Semidefinite Programming
- Semilinear Programming

Discrete and Integer Optimization

- Combinatorial Optimization
 - Traveling Salesman Problem
- Integer Programming
 - Mixed Integer Linear Programming
 - Mixed Integer Nonlinear Programming

Optimization Under Uncertainty

- Robust Optimization
- Stochastic Programming
 - Chance Constrained Optimization
- Simulation/Noisy Optimization
- Stochastic Algorithms

Complementarity Constraints and Variational Inequalities

- Complementarity Constraints
- Game Theory
- Linear Complementarity Problems
- Mathematical Programs with Complementarity Constraints
- Nonlinear Complementarity Problems

Systems of Equations and Inequalities

- Data Fitting/Robust Estimation
- Nonlinear Equations
- Nonlinear Least Squares

Multiobjective Programming

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About NEOS



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- QPLIB: 367 instances

<http://qplib.zib.de/>

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- Exactly reformulate nonlinear term, if possible
- Several tailored methods for convex MINLPs (not exact for nonconvex MINLPs)
- Identifying convexity is, in general, very difficult

Outline

- 1 Motivating Applications
- 2 Mathematical Programming Formulations
- 3 Reformulations and Relaxations
- 4 Convex MINLP
 - Branch-and-Bound
 - Outer-Approximation
 - Generalized Benders Decomposition
 - Extended Cutting Plane
 - LP/NLP-based Branch-and-Bound
 - Hybrid Algorithms
- 5 Convex functions and properties
- 6 Practical Tools
- 7 Tomorrow: nonconvex MINLPs

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

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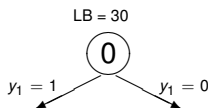
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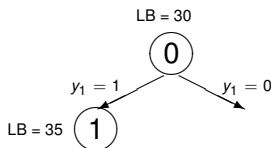
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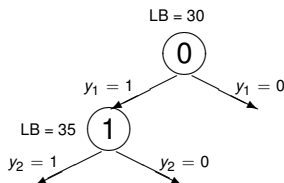
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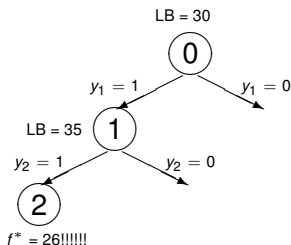
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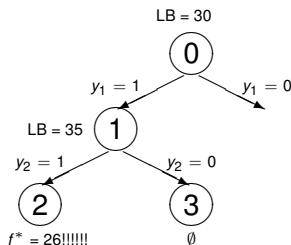
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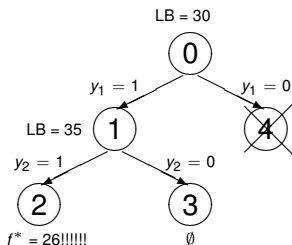
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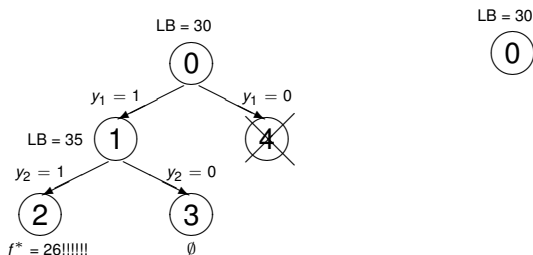
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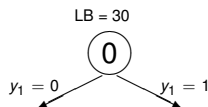
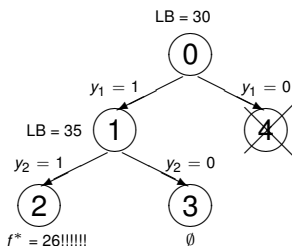
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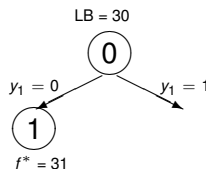
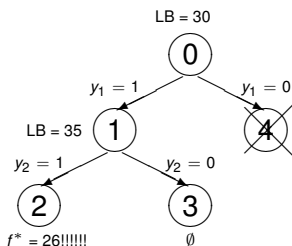
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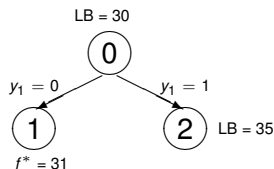
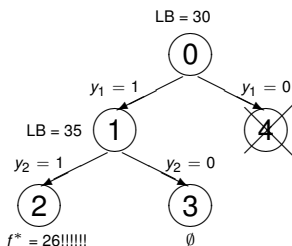
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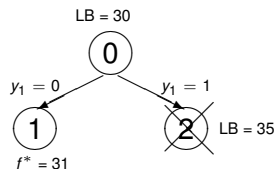
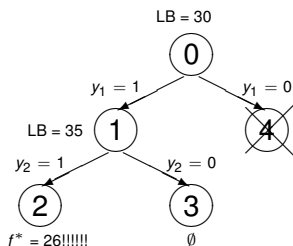
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Outer Approximation and nonconvex MINLPs

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) .

