Programmation Mathématique Avancée: Mixed Integer Nonlinear Programming

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LIX, CNRS & École Polytechnique

MPRO – PMA

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

General Information about PMA

Lecturers:

- **Amélie Lambert** (CNAM): Quadratic Programming (3 lectures)
- **Claudia D'Ambrosio, responsable du cours** (CNRS & École Polytechnique): convex and nonconvex Mixed Integer Nonlinear Programming (2 lectures)

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

General Information about PMA

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Exam:

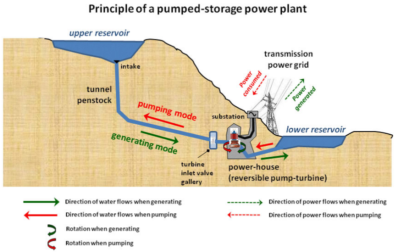
- documents/material allowed
- 2 parts, one per lecturer
- 2 hours (**Starts at 9:30 am**)

Outline

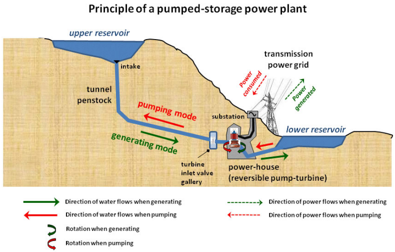
Outline

Motivating Applications

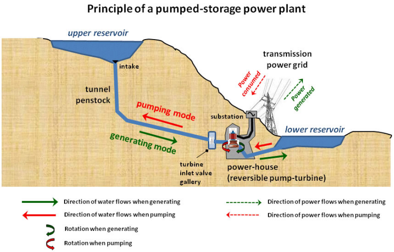
Motivating Applications

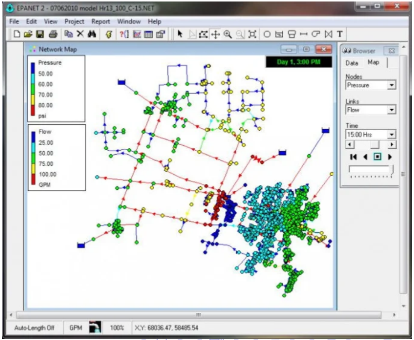


Motivating Applications



Motivating Applications





Robust Portfolio Selection

Robust Portfolio Selection

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

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

where $\overline{\Sigma} \in \mathbb{R}^{n \times n}$ 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.

Outline

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

(MINLP)

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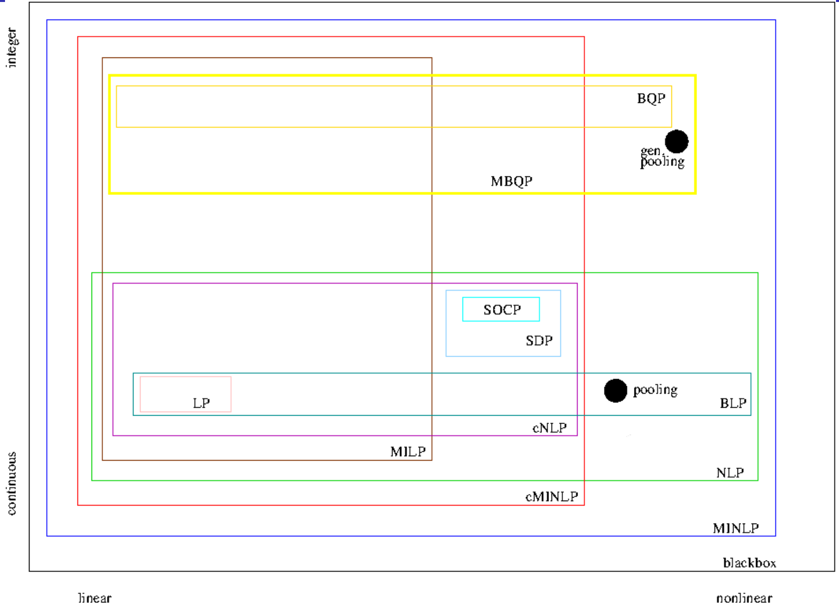
Hypothesis: f and g are twice continuously differentiable functions.

Main optimization problem classes



Outline

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.

Complexity

Theorem [Jeroslow, 1973]
The problem of minimizing a linear form over quadratic constraints in integer variables is not computable by a recursive function.

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

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

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.
- A. Del Pia, S.S. Dey, M. Molinaro, Mixed-integer quadratic programming is in NP, **Mathematical Programming A**, 162(1), pp. 225–240, 2017.

Outline

Exact reformulations

(MINLP')

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

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

Exact reformulations

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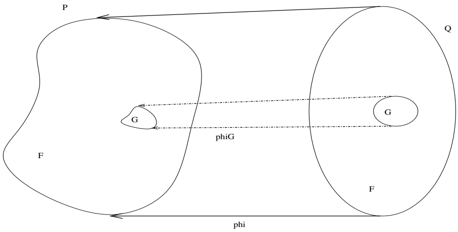
The formulation (MINLP') is an **exact reformulation** of (MINLP) if

- $\forall (w',z')$ 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')

(MINLP')

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

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 $q = q_1 + q_2$.



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

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

or

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

Exact reformulations: example 2

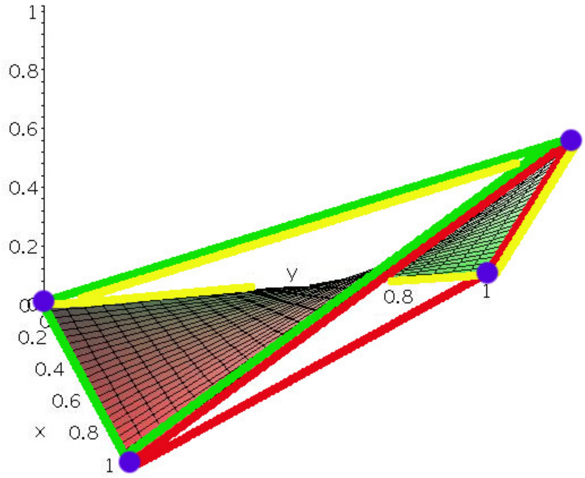
xy when *y* is binary

- 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:

$$
\begin{aligned}
w &\geq 0 \\
w &\geq x + y - 1 \\
w &\leq x \\
w &\leq y
\end{aligned}
$$

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

“Proof”



“Proof”

$$
\begin{aligned}
w &\geq 0\\
w &\geq x + y - 1\\
w &\leq x\\
w &\leq y
\end{aligned}
$$

$$
\begin{aligned}
y &= 0\\
\hline
w &\geq 0\\
w &\geq x - 1\\
w &\leq 0\\
w &\leq x
\end{aligned}
$$

$w = 0$

$$
\begin{aligned}
y &= 1\\
\hline
w &\geq 0\\
w &\geq x\\
w &\leq 1\\
w &\leq x
\end{aligned}
$$

$w = x$

Relaxations

(rMINLP)

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

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

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:

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

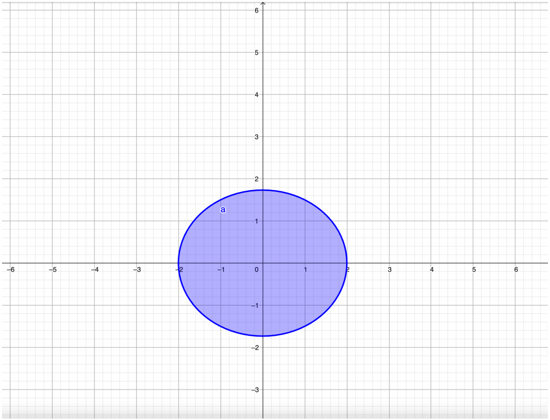
- These are called **McCormick's envelopes**
- Get an LP relaxation (solvable in polynomial time)

References & Software

- Fortet, *Applications de l'algèbre de Boole en recherche opérationelle*, **Revue Française de Recherche Opérationelle**, 4, pp. 251–259, 1960.
- McCormick, *Computability of global solutions to factorable nonconvex programs: Part I — Convex underestimating problems*, **Mathematical Programming**, 1976.
- Liberti, *Reformulations in Mathematical Programming: definitions and systematics*, **RAIRO-RO**, 2009.
- Liberti, Cafieri, Tarissan, *Reformulations in Mathematical Programming: a computational approach*, in Abraham et al. (eds.), **Foundations of Comput. Intel.**, 2009
- ROSE (`https://projects.coin-or.org/ROSE`)

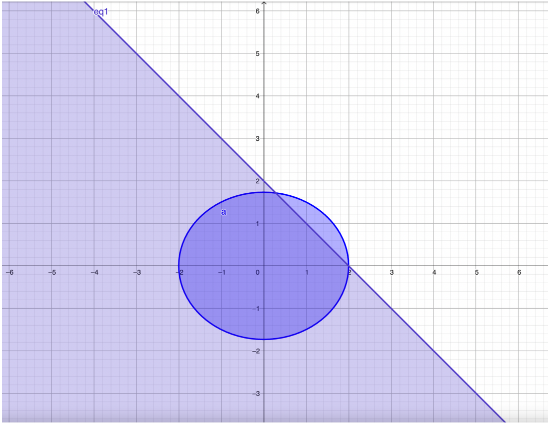
Outline

Numerical example: Convex NLP



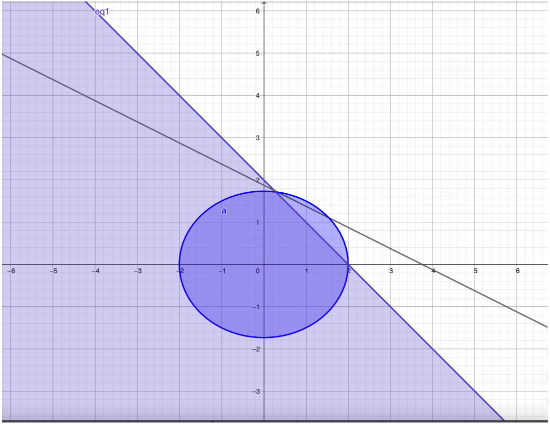
$$3x_1^2 + 4x_2^2 \leq 12$$

Numerical example: Convex NLP



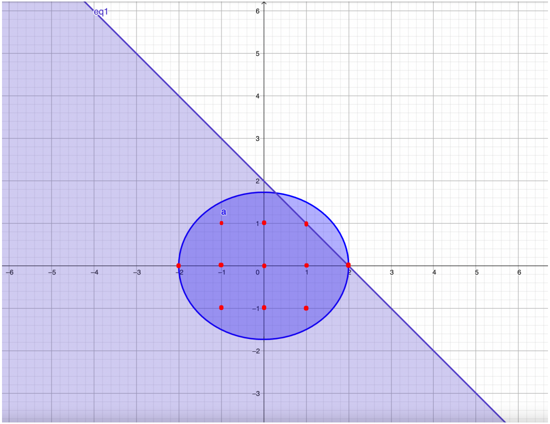
$$3x_1^2 + 4x_2^2 \leq 12$$
$$x_1 + x_2 \leq 2$$

Numerical example: Convex NLP



$$\max x_1 + 2x_2$$
$$3x_1^2 + 4x_2^2 \leq 12$$
$$x_1 + x_2 \leq 2$$

Numerical example: Convex MINLP



$$\max y_1 + 2y_2$$
$$3y_1^2 + 4y_2^2 \leq 12$$
$$y_1 + y_2 \leq 2$$
$$y_1, y_2 \in \mathbb{Z}$$

What is a convex MINLP?

Convex Mixed Integer NonLinear Programming (MINLP).

$$\begin{array}{rcl} \min f(x,y) & & \\ g(x,y) & \leq & 0 \\ x & \in & X = \{x \mid x \in \mathbb{R}^{n_1}, Dx \leq d, x^L \leq x \leq x^U\} \\ y & \in & Y = \{y \mid y \in \mathbb{Z}^{n_2}, Ay \leq a, y^L \leq y \leq y^U\} \end{array}$$

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

- continuous

What is a convex MINLP?

Convex Mixed Integer NonLinear Programming (MINLP).

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\end{array}
$$

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

* continuous
* twice differentiable

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Convex Mixed Integer NonLinear Programming (MINLP).

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$$

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

* continuous
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functions.

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Convex Mixed Integer NonLinear Programming (MINLP).

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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

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* twice differentiable
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functions.

- Local optima are also global optima .

Convex MINLP Algorithms

- Branch-and-Bound (BB).

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- Outer-Approximation (OA).

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Convex MINLP Algorithms

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Convex MINLP Algorithms

- Branch-and-Bound (BB).
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- Extended Cutting Plane (ECP).
- LP/NLP-based Branch-and-Bound (QG).
- Hybrid Algorithms (Hyb).

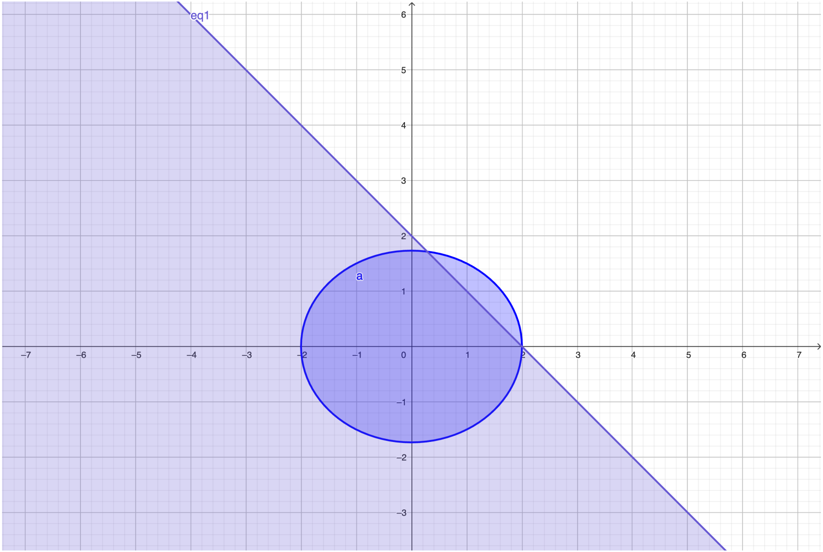
Outline

NLP relaxation

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

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)



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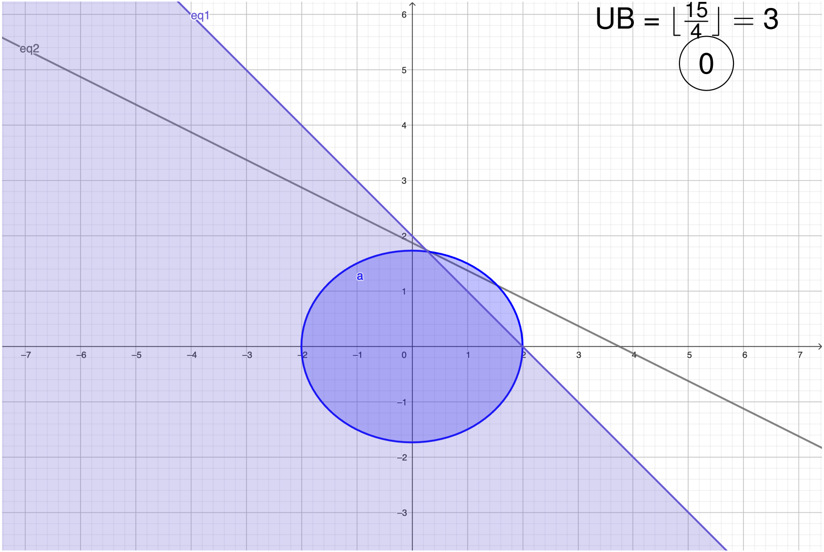

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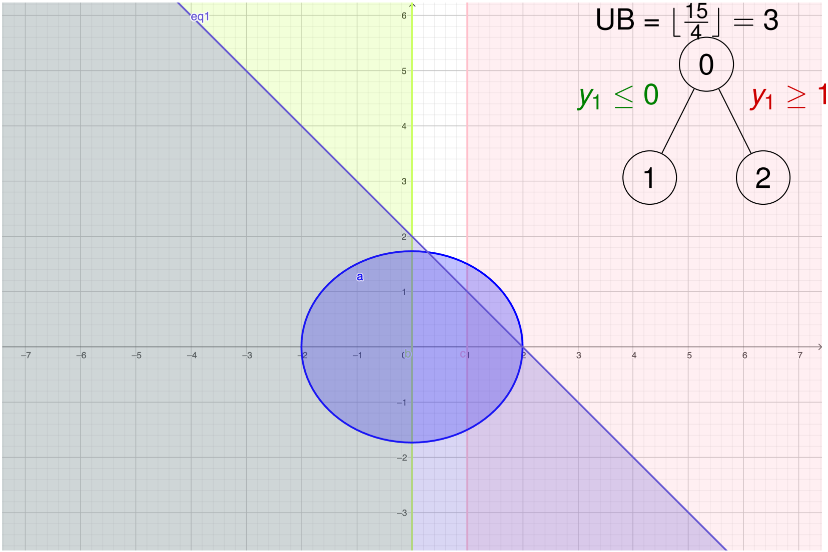

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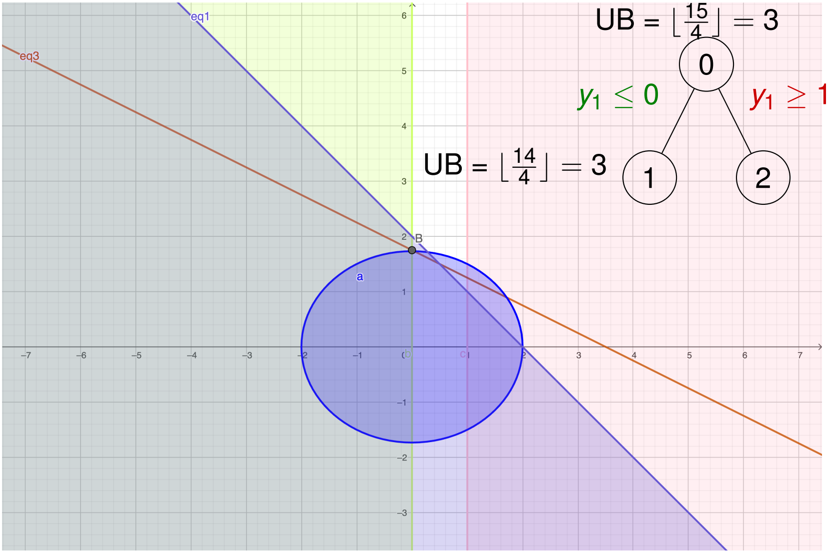

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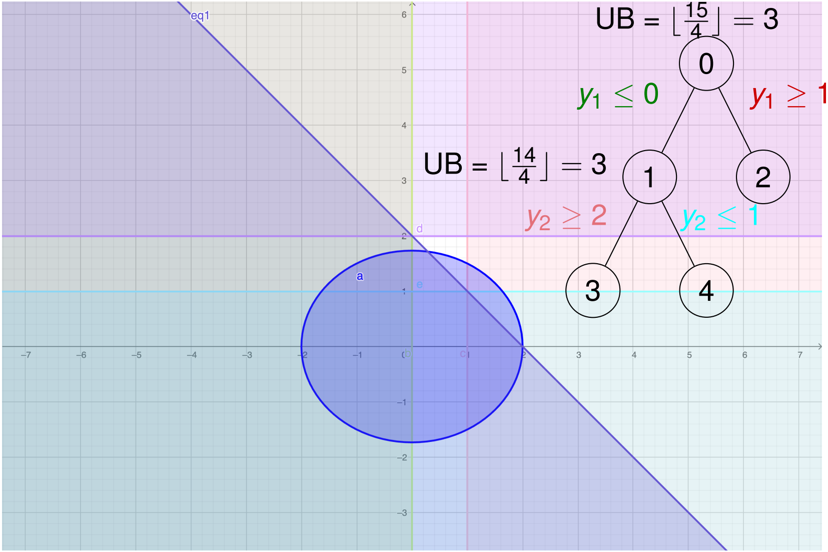

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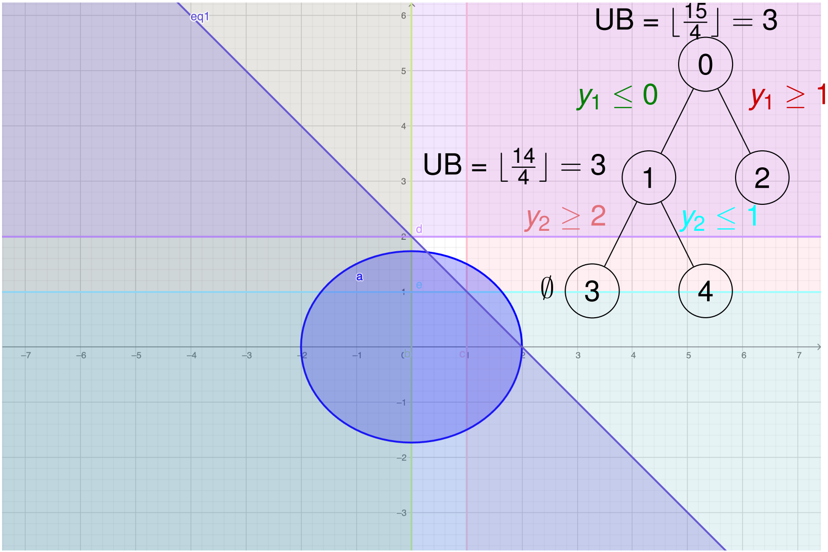
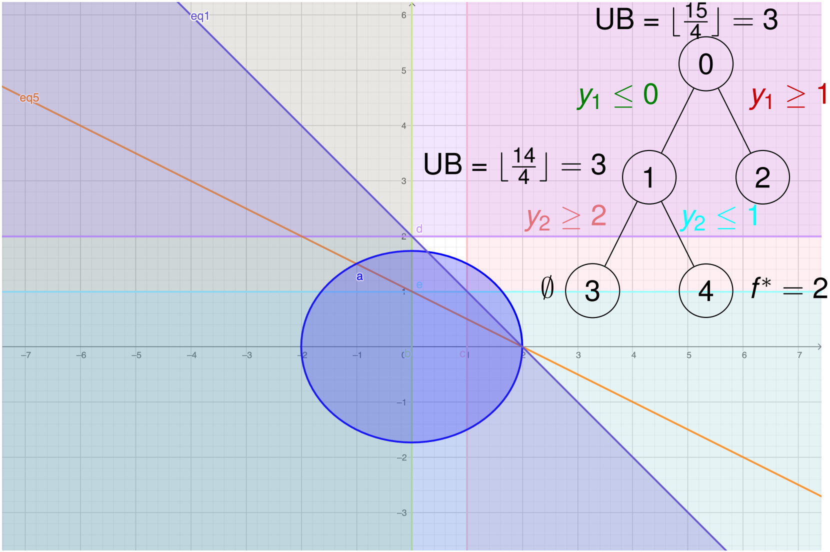
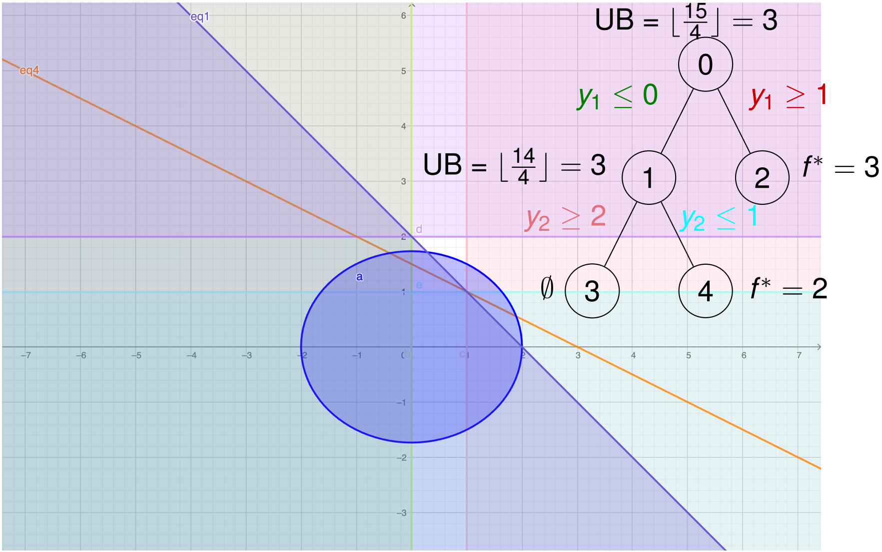




eq1
eq5
a
d
e
b
c
UB = $\lfloor \frac{15}{4} \rfloor = 3$
0
$y_1 \leq 0$
$y_1 \geq 1$
UB = $\lfloor \frac{14}{4} \rfloor = 3$
1
2
$y_2 \geq 2$
$y_2 \leq 1$
$\emptyset$
3
4
$f^* = 2$

Branch-and-Bound (BB)



Branch-and-Bound (BB)

Gupta and Ravindran, 1985. Link BB for MILPs.

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1: $f^* = +\infty$, $\Pi = \{P^0\}$, $LB(P^0) = -\infty$ where P^0 = NLP relaxation.

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Gupta and Ravindran, 1985. Link BB for MILPs.

1: $f^* = +\infty$, $\Pi = \{P^0\}$, $LB(P^0) = -\infty$ where P^0 = NLP relaxation.
2: **while** $\Pi \neq \emptyset$ **do**

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2: **while** $\Pi \neq \emptyset$ **do**
3: Choose the current subproblem $P \in \Pi$, $\Pi = \Pi \setminus \{P\}$.

Gupta and Ravindran, 1985. Link BB for MILPs.

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2: **while** $\Pi \neq \emptyset$ **do**
3: Choose the current subproblem $P \in \Pi$, $\Pi = \Pi \setminus \{P\}$.
4: Solve P obtaining $(\bar{x}, \bar{y})$.

Branch-and-Bound (BB)

Gupta and Ravindran, 1985. Link BB for MILPs.

$f^* = +\infty$, $\Pi = \{P^0\}$, $LB(P^0) = -\infty$ where P^0 = NLP relaxation.
while $\Pi \neq \emptyset$ **do**
    Choose the current subproblem $P \in \Pi$, $\Pi = \Pi \setminus \{P\}$.
    Solve P obtaining $(\bar{x}, \bar{y})$.
    if P infeasible $\vee$ $f(\bar{x}, \bar{y}) \geq f^*$ **then**
        continue
    end if

Branch-and-Bound (BB)

Gupta and Ravindran, 1985. Link BB for MILPs.

```
f* = +∞, Π = {P^0}, LB(P^0) = −∞ where P^0 = NLP relaxation.
while Π ≠ ∅ do
    Choose the current subproblem P ∈ Π, Π = Π \ {P}.
    Solve P obtaining (x̄, ȳ).
    if P infeasible ∨ f(x̄, ȳ) ≥ f* then
        continue
    end if
    if ȳ ∈ Z^{n_2} then
```

Branch-and-Bound (BB)

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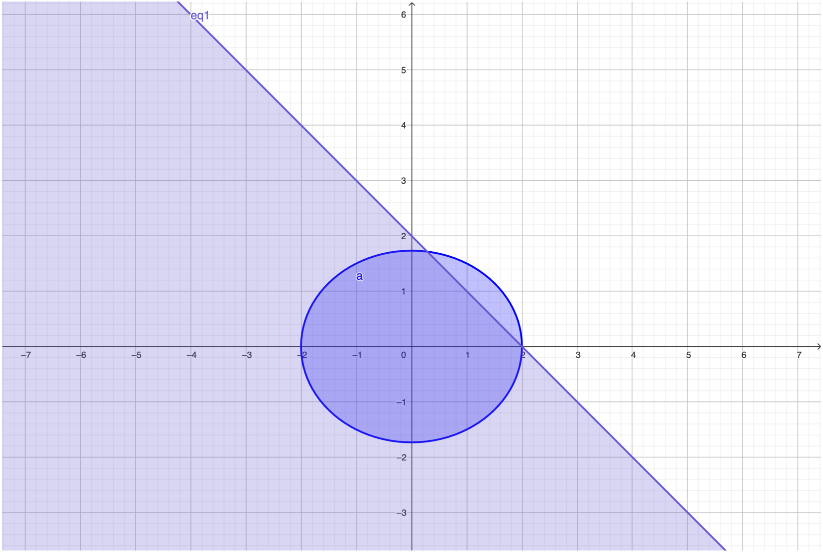
- The subproblem P^k has $LB(P^k) \geq f^*$.

How to choose the branching variables?



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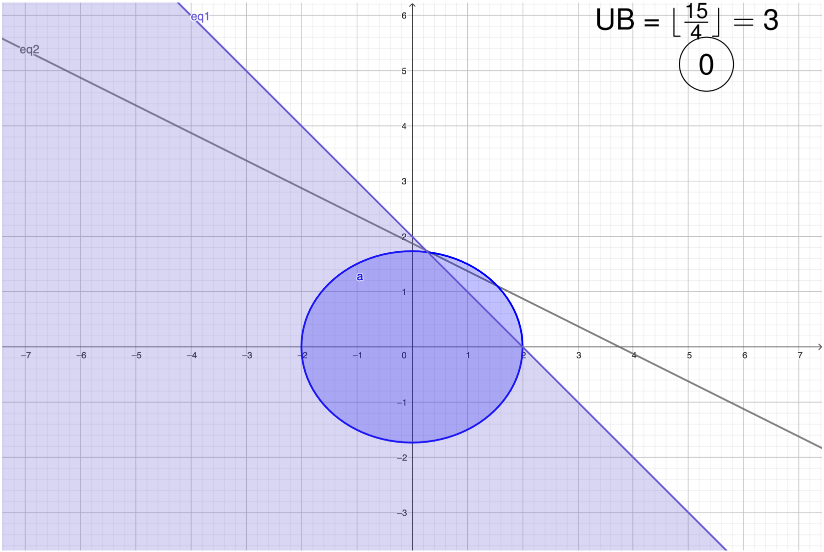

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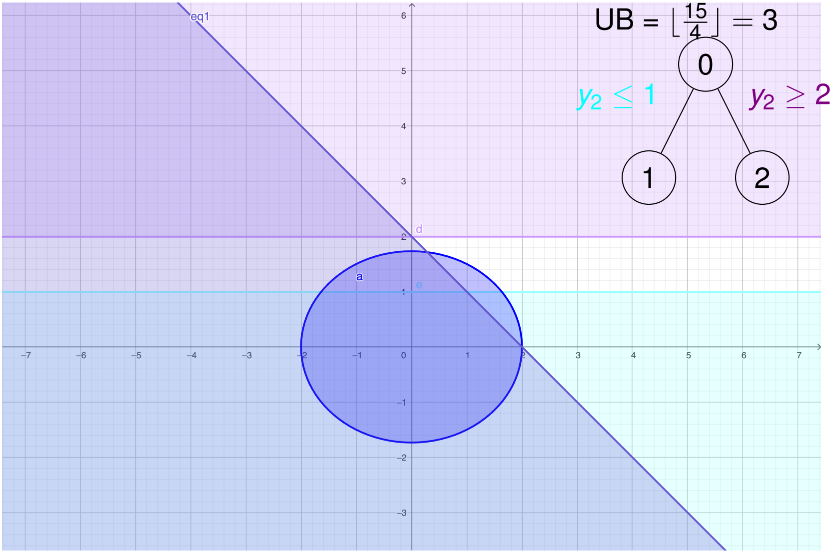

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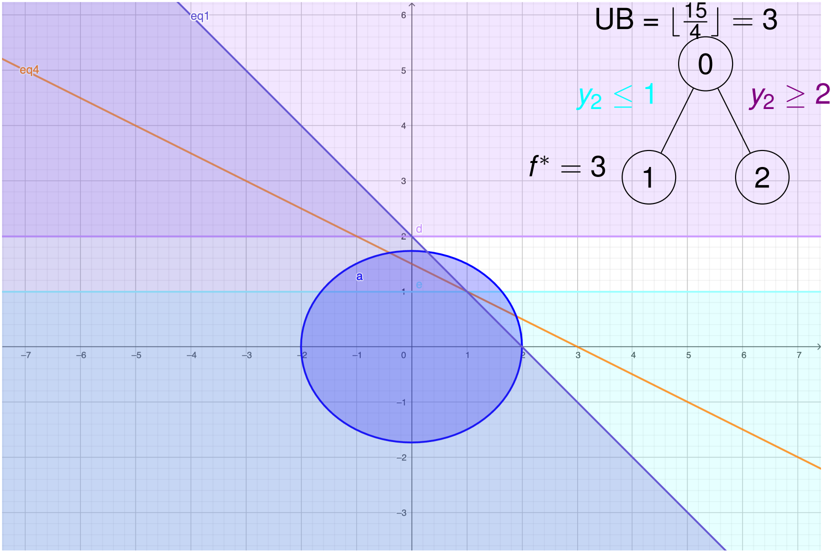

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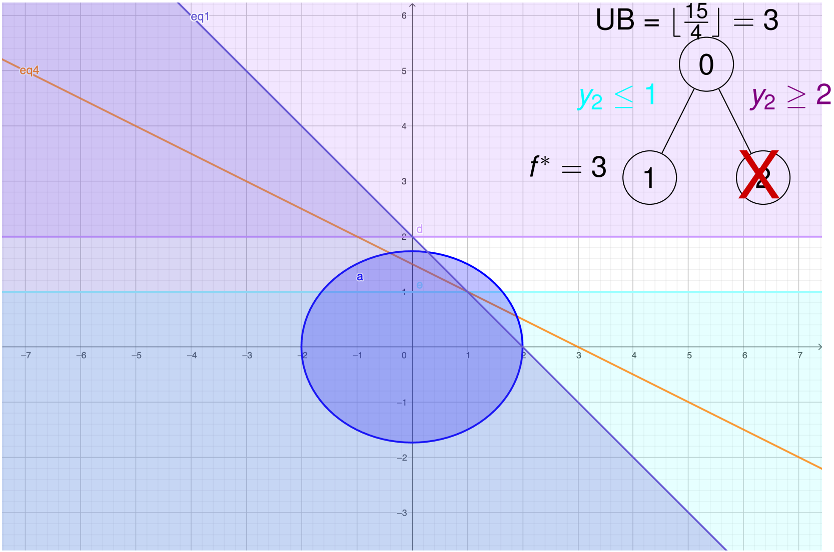

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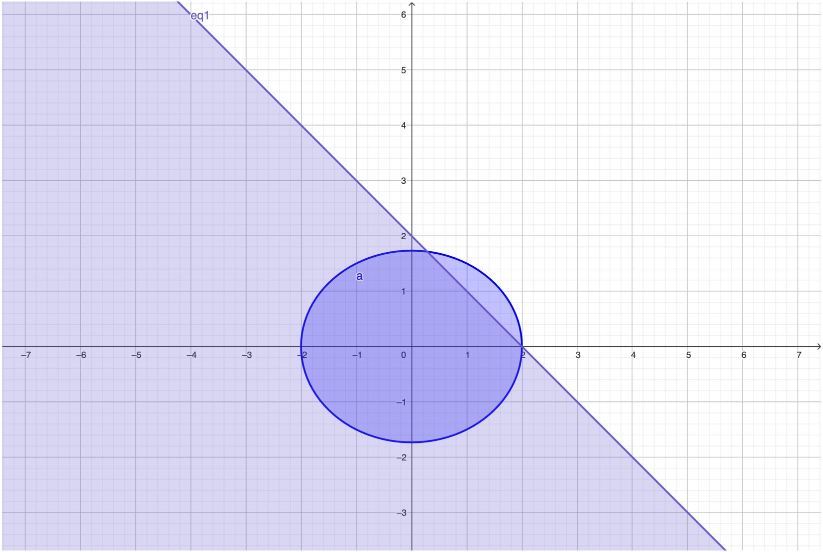

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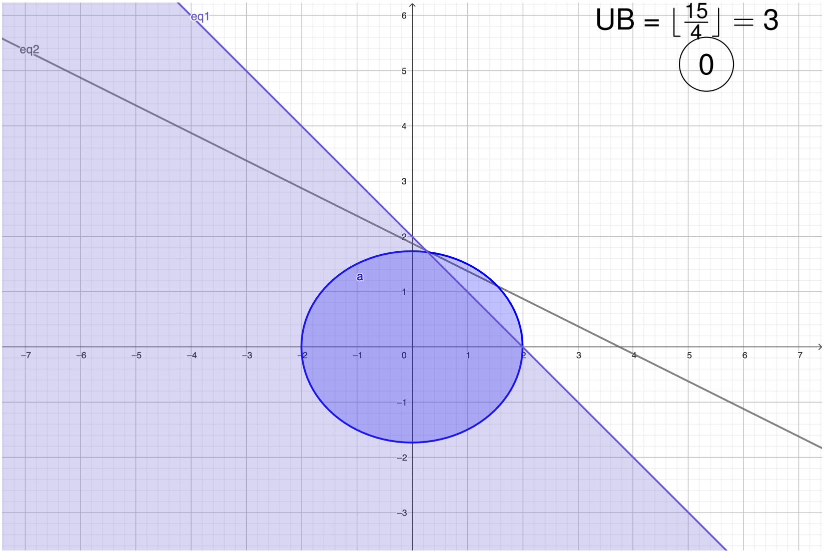

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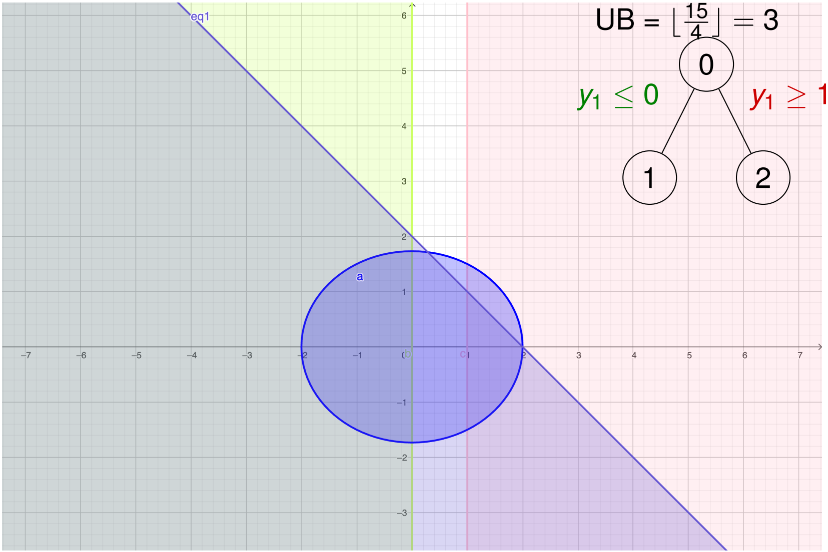

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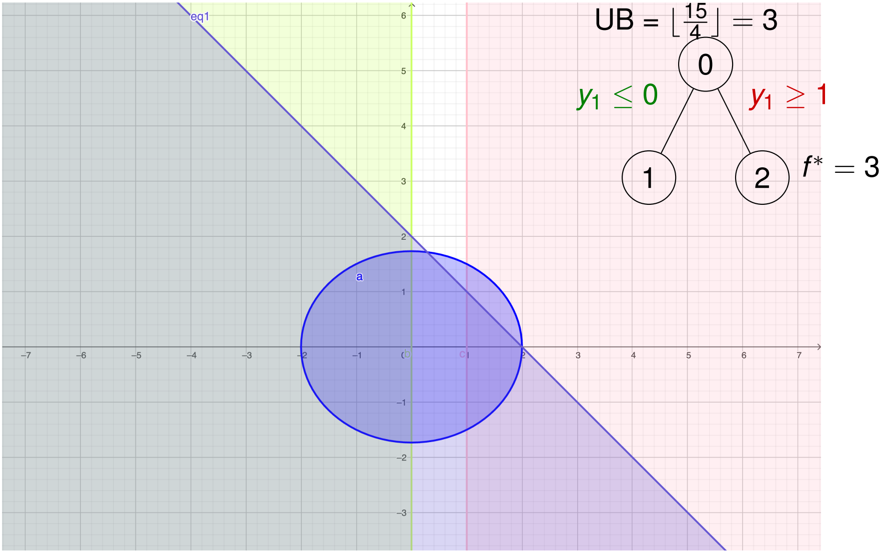

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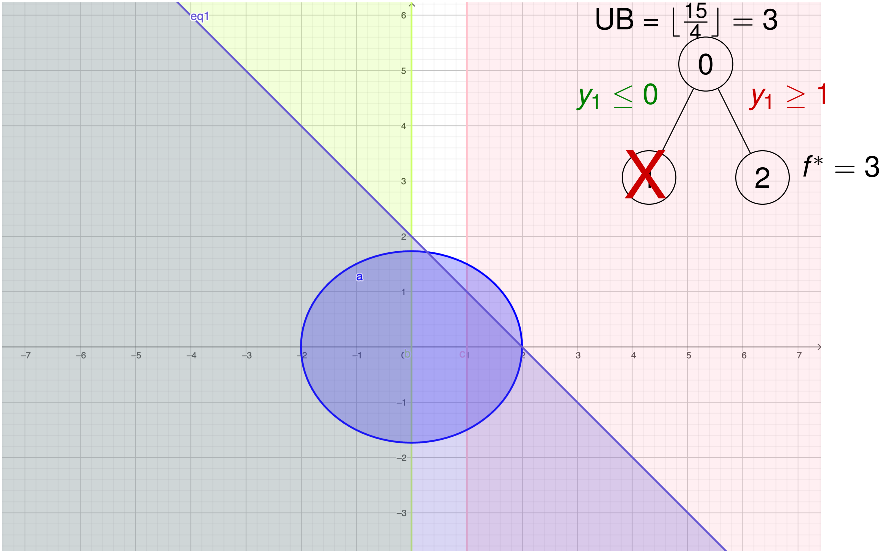

Branch-and-Bound (BB)

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

Outer-Approximation (OA)

Duran and Grossmann, 1986.

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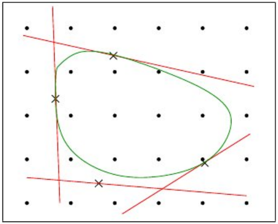

Epigraph form

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

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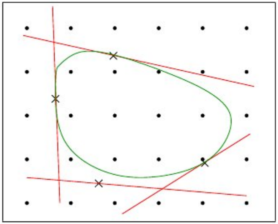

$$\min \gamma$$
$$f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} \leq \gamma \quad \forall k$$
$$g_i(x^k, y^k) + \nabla g_i(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} \leq 0 \quad \forall k \ \forall i \in I^k$$
$$x \in X$$
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$I^k = \{1, 2, \dots, m\} \ \forall k = 1, \dots, K.$

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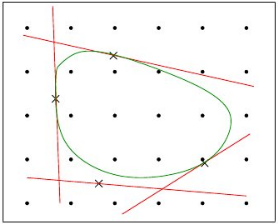

$$\begin{array}{rcll} & \min \gamma & & \\ f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} & \leq & \gamma & \forall k \\ g_i(x^k, y^k) + \nabla g_i(x^k, y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} & \leq & 0 & \forall k \; \forall i \in I^k \\ x & \in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

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

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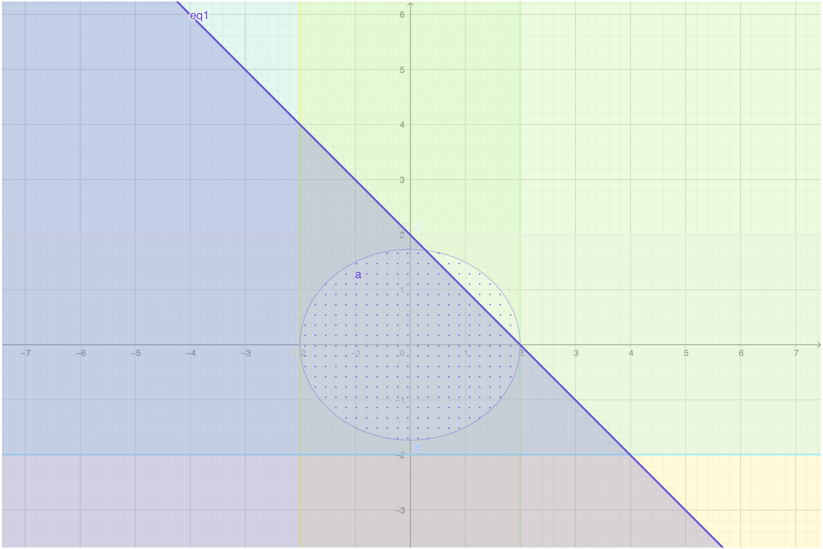

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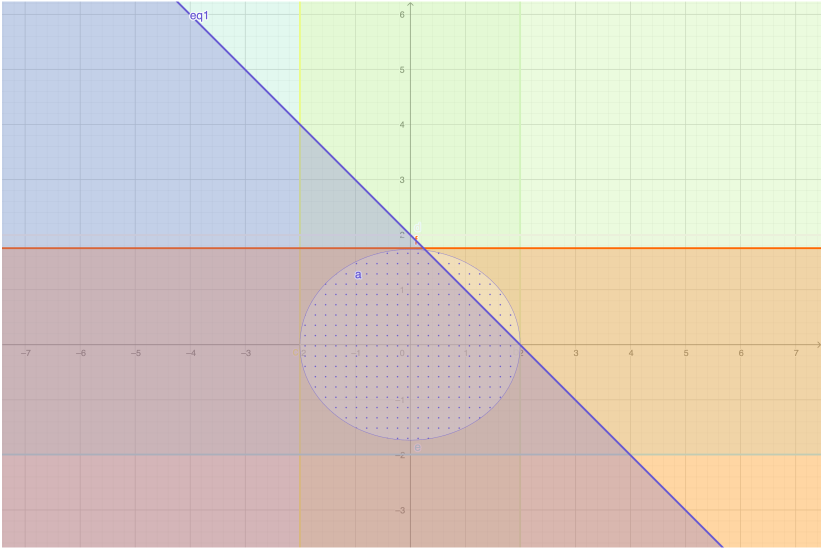

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NLP restriction and Feasibility subproblem

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

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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, Bonami, Ouorou. An Outer-Inner Approximation for separable MINLPs, INFORMS Journal on Computing (2014)

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

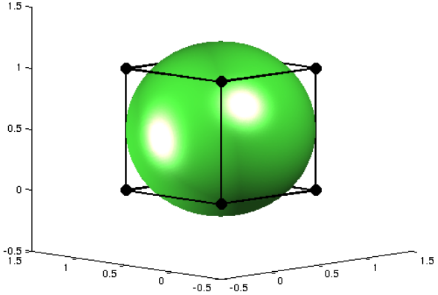

Figure: Source Belotti et al. (2013)

Outline

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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.

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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Extended Cutting Plane (ECP)

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    end if
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More iterations needed wrt OA.

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Finite convergence as for BB.

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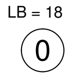

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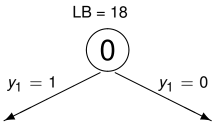

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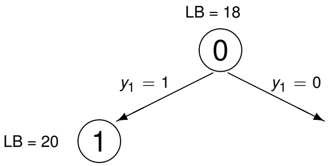

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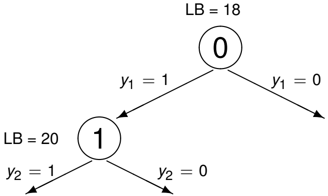

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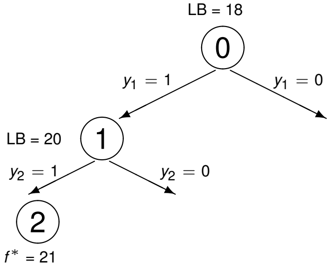

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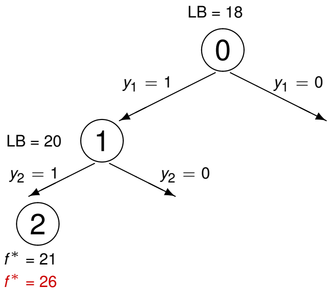

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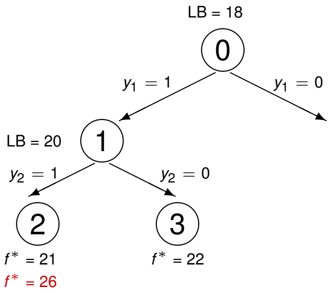

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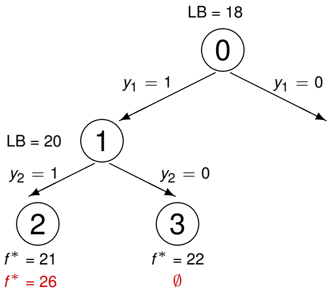

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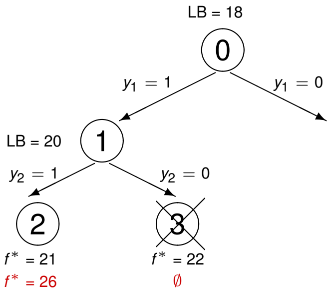

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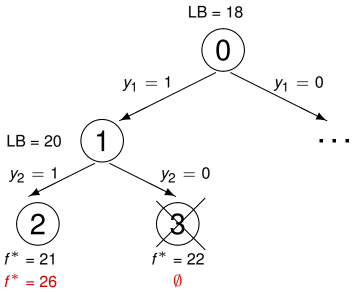

Outline

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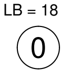

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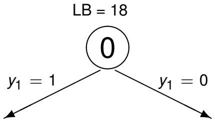

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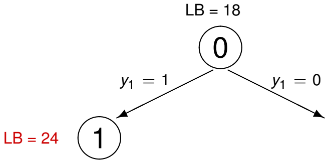

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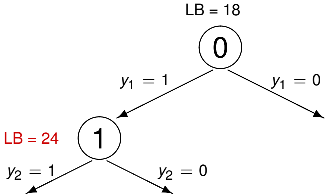

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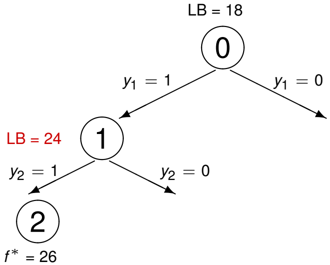

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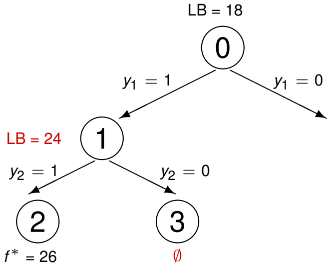

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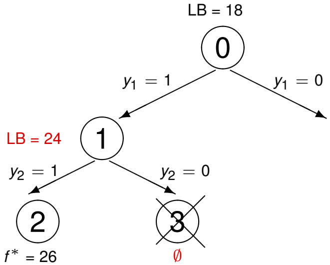

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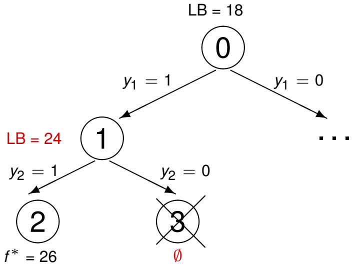

Number of subproblems solved

	# 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.

[1] weaker lower bound w.r.t. OA, MILP with less constraints than the one of OA
[2] stronger lower bound w.r.t. QG ,MILP with more constraints than the one of QG

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Outline

Reminder: Convex functions and some properties

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- Minimization, e.g., $\inf_{z \in C} f(x, z)$

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

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param Umax default 100;
param U {j in VARS};
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Neos

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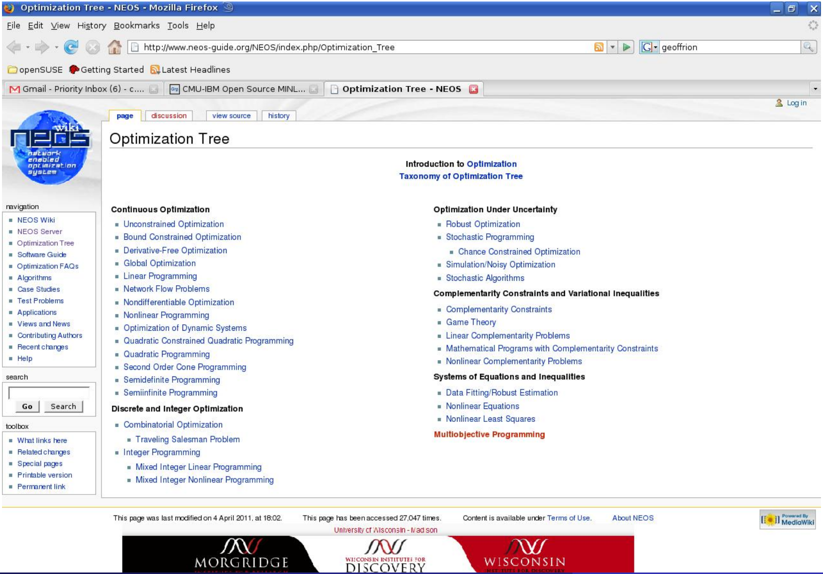

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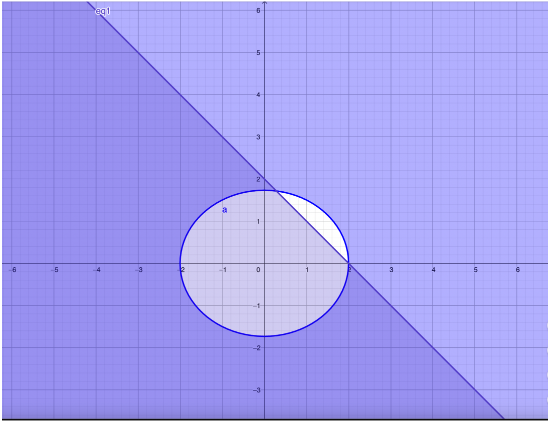
- When modeling a problem, do not forget to define simple bounds on each variable
- Exactly reformulate nonlinear term, if possible
- Several tailored methods for convex MINLPs (not exact for nonconvex MINLPs)
- Identifying convexity is, in general, very difficult

Outline

Numerical example: Convex NLP



$$3x_1^2 + 4x_2^2 \geq 12$$
$$x_1 + x_2 \leq 2$$

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.
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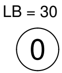

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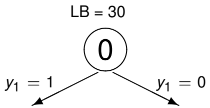

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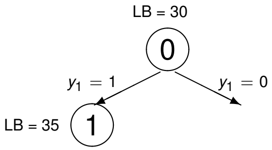

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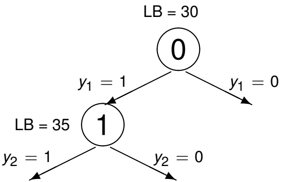

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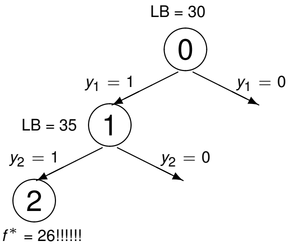

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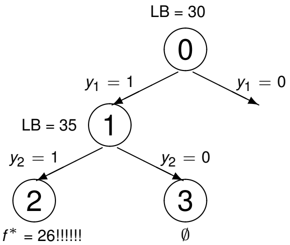

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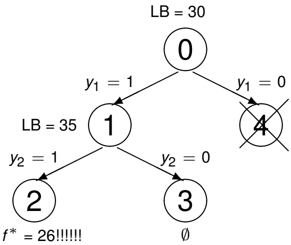

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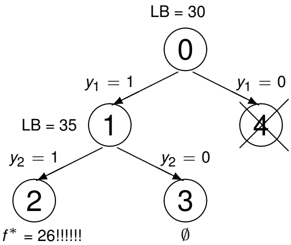

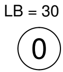

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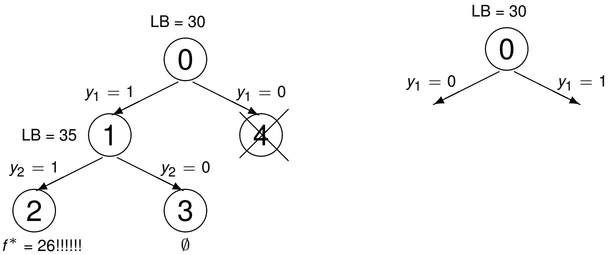

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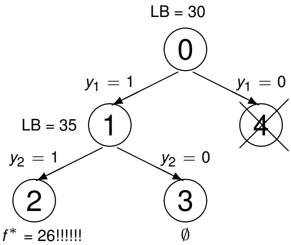

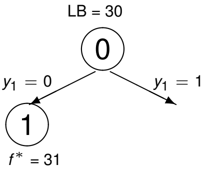

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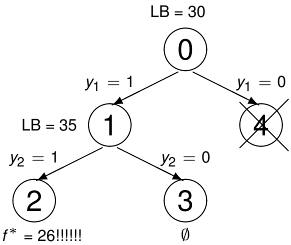

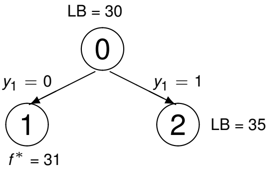

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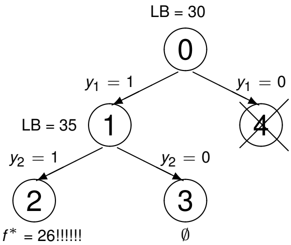

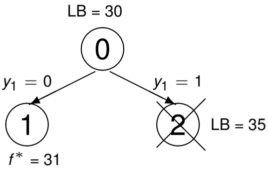

Outer Approximation and nonconvex MINLPs

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

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

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