### Optimization based on Mixed Integer Nonlinear Programming methods

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What is MP?

What is a MINLP? Subclasses of MINLP Dealing with nonconvexities

Global Optimization methods

Spatial Branch-and-Bound Expression trees Convex relaxation Variable ranges Bounds tightening

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### Outline

### What is MP?

### What is a MINLP?

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- Neos
- MINLP Libraries

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### What is Mathematical Programming?

- MP: formal language for expressing optimization problems P
  - Parameters p =problem input p also called an instance of P
  - Decision variables x: encode problem output
  - Objective function min f(p, x)
  - ► Constraints ∀i ≤ m g<sub>i</sub>(p, x) ≤ 0 f, g: explicit mathematical expressions involving symbols p, x
- If an instance p is given (i.e. an assignment of numbers to the symbols in p is known), write f(x), g<sub>i</sub>(x)

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### Main optimization problem classes



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

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

\* continuous

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\* twice differentiable

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- \* continuous
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Local optima are not always global optima.

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with  $f(x, y) : \mathbb{R}^{p+q} \to \mathbb{R}$  and  $g(x, y) : \mathbb{R}^{p+q} \to \mathbb{R}^{m}$ .

Subclasses :

- \* f and g are convex: convex MINLPs.
- \* f and g are separable: separable MINLP.
- \* f and g are quadratic: quadratic MINLP.
- \* f and g are polynomial: polynomial MINLP.

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Based on:

# 1. Continuous (NLP) Relaxation: relax integrality requirements

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Based on:

- 1. Continuous (NLP) Relaxation: relax integrality requirements
- 2. (Mixed Integer) Linear Relaxation: outer approximation

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NP-hard to solve in general!

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### MINLP branch-and-bound

Branch-and-bound algorithm:

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### MINLP branch-and-bound

<u>Branch-and-bound</u> 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

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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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Different starting points for root/each node.

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Different starting points for root/each node.

LB = min(30,

0

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Different starting points for root/each node.

LB = min(30, 28,

# 0

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Different starting points for root/each node.

LB = min(30, 28, 32,

# 0

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LB = min(30, 28, 32, 30,

# (0

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Different starting points for root/each node.

LB = min(30, 28, 32, 30, 23) = 23



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Different starting points for root/each node.

LB = min(30, 28, 32, 30, 23) = 23  $y_1 = 1$   $y_1 = 0$ 

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### Different starting points for root/each node.

LB = min(30, 28, 32, 30, 23) = 23  $y_1 = 1$   $y_1 = 0$ (1)

LB = min(35,

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LB = min(30, 28, 32, 30, 23) = 23  $y_1 = 1$   $y_1 = 0$ (1)

LB = min(35, 24,

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LB = min(35, 24, 28,

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LB = min(30, 28, 32, 30, 23) = 23 0  $y_1 = 1$  $y_1 = 0$ 

LB = min(35, 24, 28, 24,

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### Different starting points for root/each node.



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### Different starting points for root/each node.



Still not a valid LB!

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

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

where  $I^k \subseteq \{1, 2, \dots, m\}$ . Two "classical" choices: •  $I^k = \{1, 2, \dots, m\}$  Claudia D'Ambrosio

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

where 
$$I^k \subseteq \{1, 2, ..., m\}$$
. Two "classical" choices:  
•  $I^k = \{1, 2, ..., m\}$   
•  $I^k = \{i \mid g(x^k, y^k) > 0, 1 \le i \le m\}$ 

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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. Claudia D'Ambrosio

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# Global Optimization methods



b: local solution of objective function in whole space

### Exact

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



### Heuristic

 Find solution with probability 1 in infinite time

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Falk and Soland (1969) "An algorithm for separable nonconvex programming problems".

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

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

- Tree-like search
- Explores search space exhaustively but implicitly
- Builds a sequence of decreasing upper bounds and increasing lower bounds to the global optimum
- Exponential worst-case
- Like BB for MILP, but may branch on continuous vars Done whenever one is involved in a nonconvex term

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

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

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

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No more subproblems left, return x<sup>\*</sup> and terminate

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# Spatial B&B: Pruning

- 1. *P* was branched into  $C_1, C_2$
- 2.  $C_1$  was branched into  $C_3$ ,  $C_4$
- 3.  $C_3$  was pruned by optimality  $(x^* \in \mathcal{G}(C_3) \text{ was found})$
- 4. *C*<sub>2</sub>, *C*<sub>4</sub> were **pruned by bound** (lower bound for *C*<sub>2</sub> worse than *f*\*)
- 5. No more nodes: whole space explored,  $x^* \in \mathcal{G}(P)$

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# Spatial B&B: Pruning

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- 5. No more nodes: whole space explored,  $x^* \in \mathcal{G}(P)$
- Search generates a tree
- Suproblems are nodes
- Nodes can be pruned by optimality, bound or infeasibility (when subproblem is infeasible)
- Otherwise, they are branched

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# 1. For arbitrary *C*, checking if it is feasible is **undecidable**

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- 1. For arbitrary *C*, checking if it is feasible is **undecidable**
- 2. How do we compute a lower bound of C?

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- 1. For arbitrary *C*, checking if it is feasible is **undecidable**
- 2. How do we compute a lower bound of C?
- 3. How do we compute an upper bound of C?

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### **Upper bounds**: *x*<sup>\*</sup> can only decrease

 Computing the global optima for each subproblem yields candidates for updating x\*

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**Upper bounds**:  $x^*$  can only decrease

- Computing the global optima for each subproblem yields candidates for updating x\*
- As long as we only update x\* when x' improves it, we don't need x' to be a *global* optimum

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**Upper bounds**:  $x^*$  can only decrease

- Computing the global optima for each subproblem yields candidates for updating x\*
- As long as we only update x\* when x' improves it, we don't need x' to be a *global* optimum
- Any "good feasible point" will do

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**Upper bounds**: *x*<sup>\*</sup> can only decrease

- Computing the global optima for each subproblem yields candidates for updating x\*
- As long as we only update x\* when x' improves it, we don't need x' to be a *global* optimum
- Any "good feasible point" will do
- Specifically, use feasible local optima

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- Let  $R_P$  be a relaxation of P such that:
  - 1. *R*<sub>P</sub> also involves the decision variables of *P* (*and perhaps some others*)

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- Let  $R_P$  be a relaxation of P such that:
  - 1. *R*<sub>P</sub> also involves the decision variables of *P* (*and perhaps some others*)
  - 2. for any range  $I = [x^L, x^U]$ ,

 $R_P[I]$  is a relaxation of P[I]

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  - 3. if I, I' are two ranges

 $I \supseteq I' \to \min R_P[I] \le \min R_P[I']$ 

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  - 3. if *I*, *I*' are two ranges

 $I \supseteq I' \to \min R_P[I] \le \min R_P[I']$ 

4. For any subproblem *C* of *P*, finding  $x \in \mathcal{G}(R_C)$  or showing  $\mathcal{F}(R_C) = \emptyset$  is efficient

Specifically,  $\bar{x} = \text{localSolve}(R_C) \in \mathcal{G}(R_C)$ 

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### Processing C when it's infeasible will make sBB slower but not incorrect

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- Processing C when it's infeasible will make sBB slower but not incorrect
- $\blacktriangleright$   $\Rightarrow$  sBB still works if we simply **never discard a potentially feasible** C

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- Use a "partial feasibility test" isEvidentlyInfeasible(P)

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- Use a "partial feasibility test" isEvidentlyInfeasible(P)
  - If isEvidentlyInfeasible(C) is true, then C is guaranteed to be infeasible, and we can discard it

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Thm: If R<sub>C</sub> is infeasible then C is infeasible

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  - If isEvidentlyInfeasible(C) is true, then C is guaranteed to be infeasible, and we can discard it
  - Otherwise, we simply don't know, and we shall process it
- Thm: If R<sub>C</sub> is infeasible then C is infeasible
- **Proof**:  $\varnothing = \mathcal{F}(R_C) \supseteq \mathcal{F}(C) = \varnothing$

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### To make an sBB work efficiently, you need further tricks

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Encode mathematical expressions in trees or DAGs

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

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Encode mathematical expressions in trees or DAGs

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



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Encode mathematical expressions in trees or DAGs

E.g. 
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- ► Identify all nonlinear terms x<sub>i</sub> ⊗ x<sub>j</sub>, replace them with a linearizing variable w<sub>ij</sub>
- Add a *defining constraint*  $w_{ij} = x_i \otimes x_j$  to the formulation
- Standard form:

 $x_1^2$ 

$$\begin{array}{cccc} \min & c^{\top}(x,w) & \leq & b \\ \text{s.t.} & A(x,w) & \leq & b \\ & w_{ij} & = & x_i \otimes_{ij} x_j \text{ for suitable } i,j \\ \text{bounds } \& & \text{integrality constraints} \end{array} \right\} \\ + x_1 x_2 \Rightarrow \left\{ \begin{array}{cccc} w_{11} + w_{12} & & \\ w_{11} = x_1^2 & & \\ w_{12} = x_1 x_2 & & \\ & & & \\ \end{array} \right. \xrightarrow{+}_{y_1 \to y_2} & \xrightarrow{+}_{y_1 \to y_2} & \xrightarrow{+}_{y_1 \to y_2} \end{array} \right\}$$

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- Standard form: all nonlinearities in defining constraints
- Each defining constraint  $w_{ij} = x_i \otimes x_j$  is replaced by two convex inequalities:
  - $w_{ij} \leq \text{overestimator}(x_i \otimes x_j)$  $w_{ii} \geq \text{underestimator}(x_i \otimes x_i)$
- Convex relaxation is not the tightest possible, but it can be constructed automatically

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Some variables may be integral

- Easier to perform symbolic algorithms
- Linearizes nonlinear terms
- Adds linearizing variables and defining constraints

CONVEX RELAXATION min  $c^{\top}(x, w)$  A(x, w) = brelax def constr  $w_i \forall i$  $w^L \le w \le w^U$ 

Each defining constraint replaced by convex under- and concave over-estimators

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

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

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- In sBB we need to tighten variable bounds at each node
- Example:
  - Optimization Based Bounds Tightening (OBBT)
- OBBT: for each variable x in P compute
  - $\underline{x} = \min\{x \mid \text{conv. rel. constr.}\}$
  - $\overline{x} = \max\{x \mid \text{conv. rel. constr.}\}$

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

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Example: Box-constrained polynomial optimization.

$$\begin{array}{lll} \min & f(x,y) \\ & x_i \in [l_i,u_i] & \forall i \in \{1,\ldots,p\} \\ & y_i \in \{l_i,\ldots,u_i\} & \forall i \in \{1,\ldots,q\} \end{array}$$

where *f* is an arbitrary polynomial of degree  $d \in \mathbb{N}$ .

Let us define n = p + q and m = the number of monomials of *f*.

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# How far can we get?

### Example: Box-constrained polynomial optimization.

n	т	scip	couenne	baron
10	10	0.33 (10)	0.08 (10)	1.34 (10)
10	20	1.43 (10)	0.44 (10)	0.89 (10)
10	30	22.05 (10)	0.81 (10)	3.08 (10)
10	40	182.85 ( 9)	4.56 (10)	26.89 (10)
10	50	774.88 (9)	16.26 (10)	54.59 (10)
10	60	447.96 (5)	22.29 (10)	53.64 (10)
10	70	679.35 (4)	11.25 (10)	126.53 (10)
10	80	1574.58 (1)	74.86 (10)	577.44 (10)
10	90	3474.68 (1)	72.41 (10)	263.55 (10)
10	100	***	51.78 ( 9)	567.50 (10)
15	15	0.19 (10)	0.15 (10)	0.44 (10)
15	30	112.57 (10)	1.98 (10)	6.67 (10)
15	45	318.58 (7)	10.49 ( 9)	125.61 (10)
15	60	879.22 (2)	117.01 (10)	556.31 (10)
15	75	***	318.52 (10)	967.85 ( 8)
15	90	***	301.10 ( 6)	1440.39 ( 3)
15	105	***	495.67 ( 6)	***
15	120	***	586.83 ( 6)	952.72 (1)
15	135	***	1673.22 ( 4)	***
15	150	***	1614.30 ( 2)	***

Table: Results for bounds [-10,10], mixed-integer variables.

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# How far can we get?

## Example: Box-constrained polynomial optimization.

n	т	scip	couenne	baron
20	20	0.51 (10)	0.33 (10)	0.86 (10)
20	40	707.09 (8)	12.50 (10)	113.98 (10)
20	60	***	383.20 (10)	1842.67 ( 6)
20	80	***	1141.59 (7)	***
20	100	***	1110.76 (2)	***
20	120	***	1984.69 (1)	***
20	140	***	***	***
20	160	***	1223.26 (1)	***
20	180	***	***	***
20	200	***	***	***
25	25	2.15 (10)	0.80 (10)	2.92 (10)
25	50	1233.17 (1)	51.20 (10)	606.13 ( 9)
25	75	***	1237.38 ( 6)	3378.23 (1)
25	100	***	1167.83 (1)	***
25	125	***	***	***
25	150	***	***	***
25	175	***	***	***
25	200	***	***	***
25	225	***	***	***
25	250	***	***	***

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Table: Results for bounds [-10,10], mixed-integer variables.

 $\min(((x_0 * x_2) * (-0.47373 * y_7)) + ((0.218418 * y_7) * (x_4 * (x_0 * x_1))) +$  $((0.843784 * y_6) * (x_3 * (x_0 * x_2))) + (0.914311 * (y_0 * (y_5 * y_6))) +$  $(x_2 * (-0.620254 * (y_5 * y_8))) + ((x_0 * x_4) * (0.103064 * (y_7 * y_8))) +$  $(x_2 * (-0.300792 * (y_9 * (y_5 * y_7)))) + ((-0.788548 * y_7) * (x_1 * (x_2^2))) +$  $((x_1 * x_2) * (-0.185507 * (y_6^2))) + (x_1 * (0.428212 * (y_6^2))))$  $x_0 \in [0, 1]$  $x_1 \in [0, 1]$  $x_2 \in [0, 1]$  $x_3 \in [0, 1]$  $x_4 \in [0, 1]$ V5 binary V6 binary y7 binary V<sub>8</sub> binary y<sub>9</sub> binary

Problem size before reformulation: 10 variables (5 integer), 0 constraints.

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# Example...

	14/1 11 14/000
min w <sub>34</sub>	What is MP?
$x_0 \in [0, 1]$	What is a MINLP?
$x_1 \in [0, 1]$	Subclasses of MINLP
$x_2 \in [0, 1]$	Dealing with nonconvexitie
$x_0 \in [0, 1]$	Global
x; c [0, 1]	Optimization
x₄ ∈ [0, 1]	methous
y <sub>5</sub> binary	Spatial
y <sub>6</sub> binary	Branch-and-Bound
y7 binary	Expression trees
v <sub>e</sub> binary	Convex relaxation
y bipary	Bounds tightening
yg billary	
$w_{10} := (x_0 * x_2) \in [0, 1]$	References
$w_{11} := (y_7 * w_{10}) \in [0, 1]$	
$w_{12} := (x_0 * x_1) \in [0, 1]$	
$w_{13} := (x_4 * w_{12}) \in [0, 1]$	Practical Tools
$w_{14} := (y_7 * w_{13}) \in [0, 1]$	MINLP Solvers
$w_{15} := (x_3 * w_{10}) \in [0, 1]$	Modeling Languages
$W_{16} := (V_6 * W_{15}) \in [0, 1]$	MINLP Libraries
$Z_{17} := (V_{1} * V_{2})$ binary	Smart Gride
	Smart Grius
$z_{18} := (y_9 * z_{17})$ binary	
$w_{19} := (x_2 * y_5) \in [0, 1]$	

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# Example...

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#### min w<sub>3</sub>4

$$\begin{split} w_{20} &:= (y_8 * w_{19}) \in [0, 1] \\ w_{21} &:= (x_0 * x_4) \in [0, 1] \\ w_{22} &:= (y_7 * w_{21}) \in [0, 1] \\ w_{23} &:= (y_8 * w_{22}) \in [0, 1] \\ w_{24} &:= (y_7 * w_{19}) \in [0, 1] \\ w_{25} &:= (y_9 * w_{24}) \in [0, 1] \\ w_{26} &:= (x_2^2) \in [0, 1] \\ w_{26} &:= (x_2^2) \in [0, 1] \\ w_{27} &:= (x_1 * y_7) \in [0, 1] \\ w_{28} &:= (w_{26} * w_{27}) \in [0, 1] \\ w_{30} &:= (x_1 * x_2) \in [0, 1] \\ w_{31} &:= (z_{29} * w_{30}) \in [0, 1] \\ w_{31} &:= (z_{29} * w_{30}) \in [0, 1] \\ w_{33} &:= (x_1 * x_{22}) \in [0, 1] \\ w_{33} &:= (x_1 * x_{22}) \in [0, 1] \\ w_{34} &:= (-0.47373 * w_{11} + 0.218418 * w_{14} + 0.843784 * w_{16} + 0.914311 * z_{18} - 0.620254 * w_{20} + 0.103064 * w_{23} - 0.300792 * w_{25} - 0.788548 * w_{28} - 0.185507 * w_{31} + 0.428212 * w_{33}) \in [-2.36883, 2.50779] \end{split}$$

Problem size after reformulation: 35 variables (9 integer), 0 constraints. 🗇 🦻 🗧 👘 🚊 👘 🖉 🖉

# Outline

Subclasses of MINLP Dealing with nonconvexities Expression trees Convex relaxation Variable ranges Practical Tools Modeling Languages Neos

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### Need to evaluate function, its first and its second derivative at $(x^*, y^*)$ .

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Need to evaluate function, its first and its second derivative at  $(x^*, y^*)$ . Possible source of errors!

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Need to evaluate function, its first and its second derivative at  $(x^*, y^*)$ . Possible source of errors! Solution? Modeling Languages!

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

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Modeling languages, e.g., AMPL and GAMS. 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};
```

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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;
var V {j in VARS} >= 0, <= U[j], integer;</pre>
```

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Modeling languages, e.g., AMPL and GAMS. 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;
var ¥ {j in VARS} >= 0, <= U[j], integer;</pre>
```

maximize Total\_Profit: sum {j in VARS} c[j]/(1+b[j]\*exp(-a[j]\*(y[j]+d[j])));

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Modeling languages, e.g., AMPL and GAMS. Example:

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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;
var V {j in VARS} >= 0, <= U[j], integer;</pre>
```

maximize Total\_Profit: sum {j in VARS} c[j]/(1+b[j]\*exp(-a[j]\*(y[j]+d[j]))); subject to KP\_constraint: sum{j in VARS} w[j]\*y[j] <= C;</pre>

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# Neos

### NEOS: http://www.neos-server.org/neos/.

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# CMU/IBM: 23 different kind of MINLP problems

http://www.minlp.org

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# CMU/IBM: 23 different kind of MINLP problems

http://www.minlp.org

# MacMINLP: 51 instances

http://wiki.mcs.anl.gov/leyffer/index.php/MacMINLP

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# CMU/IBM: 23 different kind of MINLP problems

http://www.minlp.org

# MacMINLP: 51 instances

http://wiki.mcs.anl.gov/leyffer/index.php/MacMINLP

# MINLPlib: 270 instances

http://www.gamsworld.org/minlp/minlplib.htm

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 Binary variables: on/off status of generators, batteries, etc.

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- Binary variables: on/off status of generators, batteries, etc.
- Continuous variables: produced/consumer power, etc.

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- Binary variables: on/off status of generators, batteries, etc.
- Continuous variables: produced/consumer power, etc.
- Linear and nonlinear constraints: relation between status variables and produced power variables, amount of produced/consumed power, etc.

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- Binary variables: on/off status of generators, batteries, etc.
- Continuous variables: produced/consumer power, etc.
- Linear and nonlinear constraints: relation between status variables and produced power variables, amount of produced/consumed power, etc.

S. Toubaline, P.-L. Poirion, C. D'Ambrosio, L. Liberti. Observing the state of a smart grid using bilevel programming. **COCOA 2015** (accepted). What is MP?

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# Thank you!

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