# Introduction to Mixed Integer Nonlinear Programming

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## Outline of the Seminar

Introduction and Motivation

Convexity Issues

**Correlated Problems** 

Complexity Issues

**Basic Building Blocks** 

Algorithms and Softwares

## The problem of the day

The general mixed integer nonlinear problem is

$$\mathsf{MINLP} \left\{ \begin{array}{ll} \underset{x,y}{\text{minimize}} & f(x,y) \\ \text{subject to} & g(x,y) \leq 0 \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^p \end{array} \right.$$

•  $f(x,y) : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}$ ,  $g(x,y) : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$  are smooth functions.

•  $X \subset \mathbb{R}^n$ ,  $Y \subset \mathbb{R}^p$  are polytopes including bounds on the variables.

**Extremely difficult**: Combines challenges of handling nonlinearities with combinatorial explosion of integer variables [Belotti et al., 2013].

**Extremely powerful**: "The mother of all deterministic optimization problems" [Lee, 2008].

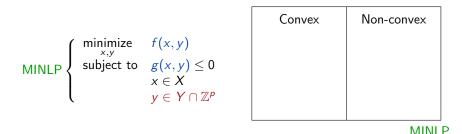
# Real-world applications [Bonami, 2014]

Application	nonlinear	discrete		
Portfolio optimization	Risk, utility, robust-	number of assets, min		
	ness	investment		
[Bienstock, 1996, Bonami and Lejeune, 2009, Vielma et al., 2008]				
Chemical plant design	Chemical reactions	what to install		
[Duran and Grossmann, 1986, Flores-Tlacuahuac and Biegler, 2007]				
Block Layout Design	Spatial constraints	what to layout		
[Castillo et al., 2005]				
Networks with delays	Delay as function of traffic	Path, flows		
[Boorstyn and Frank, 1977, Ameur and Ouorou, 2006]				
Location with	Demands	location model		
stochastic services				
[Elhedhli, 2006]				
TSP with neighbor- hoods (Robotics) [Gentilini et al., 2013]	Definition of ngbh.	TSP		

# Real-world applications [Bonami, 2014]

Application	nonlinear	discrete		
Petrochemical	Blending, pooling	Which process		
[Haverly, 1978]				
Gaz/Water networks	Pressure loss	Network topology		
[Bragalli et al., 2011]				
Nuclear Reactor	reactions	What to reload		
reloading				
[Quist et al., 1999]				
Airplane trajectory	aerodynamics	waypoints, colision		
optimization		avoidance,		
[Cafieri and Durand, 2013, Soler et al., 2013]				
Mixed Integer Opti-	DE	discrete controls		
mal control				
[Sager, 2005, 2012]				
Countless more				
see for example [Belotti et al., 2013]				

# Convexity of Nonlinear Functions

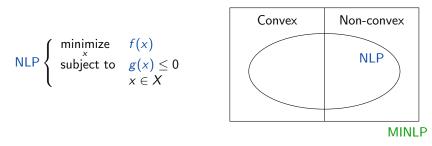


**Definition**. A smooth function  $f : \mathbb{R}^n \to \mathbb{R}$  is convex, iff for all couples of points  $x^0, x^1 \in \mathbb{R}^n$ , we have

$$f(x^1) \ge f(x^0) + \nabla f(x^0)^T (x^1 - x^0)$$

(In a slight abuse of notation) MINLP is convex iff f(x, y) and g(x, y) are convex functions, otherwise MINLP is nonconvex.

# Nonlinear Programming



• no integer variables, but challenge of handling nonlinearities.

• Convex NLP: all the minima all global minima (if strictly convex: only one minimum) and polynomial-time interior-point methods [Nesterov and Nemirovskii, 1994].

• Nonconvex NLP: find global solution is **NP**-hard (global quadratic optimization is already **NP**-hard [Sahni, 1974]).

# $\mathsf{MINLP} \neq \mathsf{NLP}$

• Convex NLP: all the minima all global minima and polynomial-time interior-point methods [Nesterov and Nemirovskii, 1994].

 $\bullet$  A strictly convex NLP has at most one global solution, the same does not hold for MINLP.

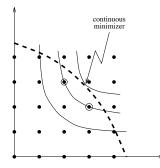
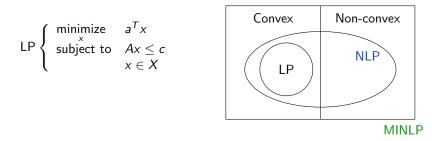


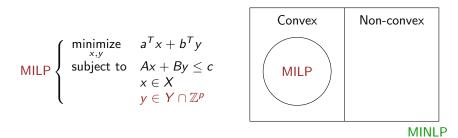
Figure: Optima for strictly convex MINLP [Leyffer, 1994].

# Linear Programming



- no integer variables, no challenge of handling nonlinearities.
- polynomial-time methods: ellipsoid algorithm [Khachiyan, 1979] and Karmarkar's algorithm [Karmarkar, 1984].
- Simplex algorithm for LP, proposed by George Dantzig in 1947, is one of the Top Ten Algorithms of the 20th Century [Dongarra and Sullivan, 2000].

# Mixed Integer Linear Programming



• linear objective function and linear constraints, but combinatorial explosion of integer variables.

• **NP**-hard problem: no known polynomial-time algorithm (0-1 integer linear programming is **NP**-complete problems [Karp, 1972]).

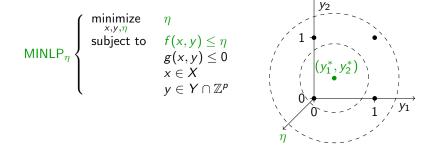
• well-studied in literature since [Gomory, 1958] and very powerful algorithms (many commercial softwares).

## Convex MINLP $\neq$ MILP

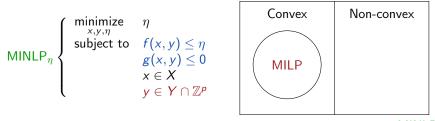
The solution of MILP is an extreme point, however the same does not hold for convex MINLP:

minimize 
$$\sum_{i=1}^{p} \left(y_i - \frac{1}{2}\right)^2$$
, subject to  $y_i \in \{0, 1\}$ ,  $i = 1, \dots, p$ 

**Trick**: Introduce a new objective function (a dummy variable  $\eta$ ) and a new constraint  $f(x, y) \leq \eta$ .



## Complexity Issues



MINLP

- MINLP is NP-hard (MILP as special case).
- In general undecidable [Jeroslow, 1973], even in "easy" case with "few" variables [De Loera et al., 2006].
- MINLP is a hot topic in optimization community: from [Leyffer, 1994] (first PhD thesis on convex MINLP) to IMA Hot Topics in 2012.

## Assumptions and Hypotheses

**Assumption 1**. All the problem function are "perfectly" known, in terms of their mathematical expression and values.

**Assumption 2**. X and Y are nonempty compact convex sets defined by systems of linear inequality constraints.

**Assumption 3**. Functions f and g are twice continuously differentiable and convex.

**Assumption 4**. MINLP $_{\eta}$  satisfies a constraint qualification condition.

- Assumptions 1: see next talk about Black Box MINLP.
- Assumptions 2 avoid undecidability problems.
- Assumptions 2 and 3  $\implies$  we consider only convex MINLP $_{\eta}$ .
- Assumptions 4: technical requirement for NLP machinery.

**Moral**: "the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity" [Rockafellar, 1993].

## Auxiliary Problems

### Relaxation in theory:

- optimize over a larger feasible region (ignore several constraints).
- compute a Lower Bound on the "real" minimum value.

**Definition**. An optimization problem  $\min{\{\tilde{f}(z) : z \in \tilde{F}\}}$  is a relaxation of  $\min{\{f(z) : z \in F\}}$ , iff  $\tilde{F} \supset F$  and  $\tilde{f}(z) \leq f(z)$  for all  $z \in F$ .

### Relaxation in practice:

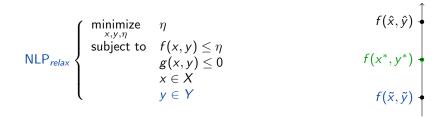
- relax integrality requirements: obtain an NLP.
- relax nonlinear constraints: obtain an MILP.

### Upper bound:

• any feasible point provides an objective value greater (or equal) that the minimum one.

 $f(\hat{x}, \hat{y}) \bullet$  $f(x^*, y^*) \bullet$  $\tilde{f}(\tilde{x}, \tilde{y}) \bullet$ 

Relax Integrality: NLP<sub>relax</sub>

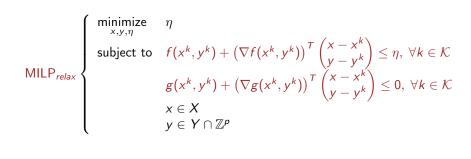


- Relax integrality: from  $y \in Y \cap \mathbb{Z}^p$  to  $y \in Y \subset \mathbb{R}^p$ .
- If MINLP<sub> $\eta$ </sub> is convex then NLP<sub>relax</sub> is convex too (globally solvable).

• If  $(\tilde{x}, \tilde{y})$  is optimal for NLP<sub>relax</sub> and feasible for MINLP<sub> $\eta$ </sub>, then it is also a minimum for MINLP<sub> $\eta$ </sub>.

• If  $(\hat{x}, \hat{y})$  is feasible for MINLP $_{\eta}$  and  $f(\hat{x}, \hat{y}) = f(\tilde{x}, \tilde{y})$ , then it is also a minimum for MINLP $_{\eta}$ .

Relax Convex Nonlinearities: MILP<sub>relax</sub>



• Relax convex nonlinearities: supporting hyperplanes at points  $(x^k, y^k)$  for  $k \in K$  (apply the definition of nonlinear convex function).

- Polyhedral (linear) relaxation of nonlinear convex constraints.
- Same relationships between solutions of  $\text{MILP}_{relax}$  and  $\text{MINLP}_{\eta}$ .

# Relaxation in pictures

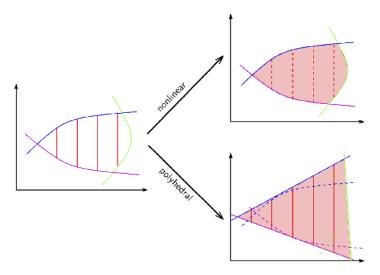
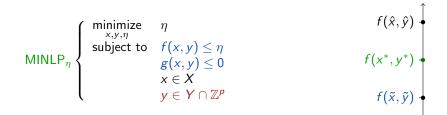


Figure: Nonlinear and polyhedral relaxation [Belotti et al., 2013].

## Constraint Enforcement



**Goal**: Exclude a solution  $(\tilde{x}, \tilde{y})$  of a relaxation, infeasible for of MINLP<sub> $\eta$ </sub>.

- Relaxation refinement: tighten the MILP<sub>relax</sub> relaxation.
- Branching: exclude set of non-integer points from NLP<sub>relax</sub>.
- Combinations of these two constraint enforcement approaches.

## Constraint Enforcement: Refinement

**Definition**. A valid inequality is an inequality that is satisfied by all feasible solutions of  $MINLP_{\eta}$ . A cut is valid inequality that "cuts off" the current point  $(\tilde{x}, \tilde{y})$  infeasible for  $MINLP_{\eta}$ .

**Example**. If  $g(x, y) \leq 0$  convex and there is an index j such that  $g_j(\tilde{x}, \tilde{y}) > 0$ , then  $(\tilde{x}, \tilde{y})$  is "cut off" by

$$g_j(\tilde{x}, \tilde{y}) + \nabla g_j(\tilde{x}, \tilde{y})^T \begin{pmatrix} x - \tilde{x} \\ y - \tilde{y} \end{pmatrix} \leq 0$$

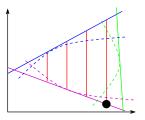


Figure:  $(\tilde{x}, \tilde{y})$  infeasible for MINLP<sub> $\eta$ </sub> [Belotti et al., 2013].

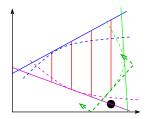


Figure: Valid inequality "cuts off"  $(\tilde{x}, \tilde{y})$ [Belotti et al., 2013].

## Constraint Enforcement: Branching

**Goal**: Exclude a fractional solution  $(\tilde{x}, \tilde{y})$  of NLP<sub>relax</sub>.

- Select fractional  $\tilde{y}_i$  for some  $i = 1, \ldots, p$ .
- Create two new sub-problems by respectively adding:

 $y_i \leq \lfloor \tilde{y}_i \rfloor$  and  $y_i \leq \lceil \tilde{y}_i \rceil$ 

 $\bullet$  Solution to  $\mathsf{MINLP}_\eta$  lies in one of the new subproblems.

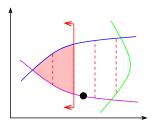


Figure: NLP subproblem with  $y_i \leq \lfloor \tilde{y}_i \rfloor$  [Belotti et al., 2013].

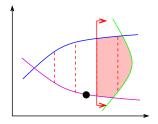
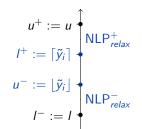


Figure: NLP subproblem with  $y_i \ge \lfloor \tilde{y}_i \rfloor$  [Belotti et al., 2013].

## Nonlinear Branch-and-Bound

 $\mathsf{NLP}_{relax} \left\{ \begin{array}{ll} \underset{x,y,\eta}{\text{minimize}} & \eta \\ \text{subject to} & f(x,y) \leq \eta \\ g(x,y) \leq 0 \\ x \in X, \ y \in Y \\ l \leq y \leq u \end{array} \right.$ 



• solve NLP<sub>relax</sub> and find a fractional solution  $(\tilde{x}, \tilde{y})$ .

• introduce two new sub-problems NLP<sup>+</sup><sub>relax</sub> and NLP<sup>-</sup><sub>relax</sub> respectively with bounds  $(l^+, u^+) := (l, u)$  and  $(l^-, u^-) := (l, u)$ :

$$u_i^- := \lfloor \widetilde{y}_i \rfloor$$
 and  $l_i^+ := \lceil \widetilde{y}_i \rceil$ 

nodes NLP<sup>+</sup><sub>relax</sub> and NLP<sup>-</sup><sub>relax</sub> correspond to the branching sub-problems.

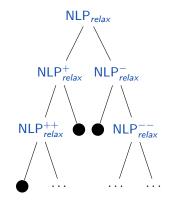
## Nonlinear Branch-and-Bound

- Iterate branching and create a tree.
- Let  $(\hat{x}, \hat{y})$  be an upper bound of MINLP<sub> $\eta$ </sub>.
- Pruning rules:

**Infeasibility**: if a sub-problem is infeasible  $\Rightarrow$  any NLP in its subtree is also infeasible.

**Integrality**: if  $(\tilde{x}, \tilde{y})$  is an integral solution (a)  $f(\hat{x}, \hat{y}) < f(\tilde{x}, \tilde{y})$ , then  $(\hat{x}, \hat{y}) := (\tilde{x}, \tilde{y})$ . (b) no better feasible solution in sub-tree.

**Dominance**: if  $f(\tilde{x}, \tilde{y}) \ge f(\hat{x}, \hat{y})$  $\Rightarrow$  no better integer solution in sub-tree.



# Nonlinear Branch-and-Bound: Pseudocode

```
initialization: set U := \infty, and add NLP<sub>relax</sub> to heap \mathcal{H}.
while \mathcal{H} \neq \emptyset do
   Remove a sub-problem from the heap \mathcal{H}.
   Find a solution (\tilde{x}, \tilde{y}) to the current sub-problem.
   if current sub-problem is infeasible then
      Prune node by infeasibility.
   else if f(\tilde{x}, \tilde{y}) > U then
      Prune node by dominance.
   else if (\tilde{x}, \tilde{y}) is integral then
      Update: U := f(\tilde{x}, \tilde{y}) and (x^*, y^*) := (\tilde{x}, \tilde{y}).
   else
      Branch on fractional variable.
```

Create two sub-problems. Add them to  $\mathcal{H}$ .

end if

end while

## Nonlinear Branch-and-Bound

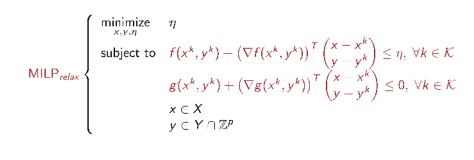
**Theorem**. All previous assumptions hold. Then Nonlinear Branch-and-Bound terminates at optimal solution (or indication of infeasibility) of MINLP<sub> $\eta$ </sub> after a finite number of iterations.

### **Open questions**:

- How to select the branching variable (maximum fractional as bad as randomly selection [Achterberg et al., 2005]).
- How to select the next sub-problem to be solved.
- Warm-starting of NLP solver.

**Goal**: Minimize size of Branch-and-Bound tree (dimension of heap  $\mathcal{H}$ ). **Strategy**: Find good upper bound and increase lower bound quickly.

# Outer Approximation [Duran and Grossmann, 1986]



- Tighten MILP<sub>relax</sub> by iteratively adding supporting hyperplanes (valid inequalities).
- Evaluate convex functions only at "integer" points  $(x^k, y^k)$  for all  $k \in \mathcal{K}$ .
- MILP machinery: more than 50 years of experience in theory and practice.

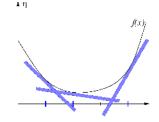


Figure: MILP<sub>relax</sub> [Leyffer, 2013].

### Outer Approximation: NLP sub-problem

$$\mathsf{NLP}_{fix} \begin{cases} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & g(x,y) \leq 0 \\ & x \in X \\ & y = \hat{y} \end{cases} \quad \mathsf{NLP}_{feas} \begin{cases} \underset{x}{\text{minimize}} & \sum_{j=1}^{m} g_{j}^{+}(x, \hat{y}) \\ \text{subject to} & x \in X \\ & \text{subject to} & x \in X \end{cases}$$

• NLP<sub>fix</sub> is feasible  $\implies$  upper bound to MINLP<sub> $\eta$ </sub>.

- NLP<sub>fix</sub> is infeasible  $\iff$  strictly positive optimal value of NLP<sub>feas</sub>.
- NLP<sub>fix</sub> is infeasible  $\implies$  nonlinear solvers provide a solution to NLP<sub>feas</sub>.

**Lemma**. Supporting hyperplanes at  $(\hat{x}, \hat{y})$  are valid inequalities for MINLP<sub> $\eta$ </sub>. If NLP<sub>*fix*</sub> is infeasible, then supporting hyperplanes are valid cut w.r.t.  $(\hat{x}, \hat{y})$ .

# Outer Approximation Algorithm

$$\mathsf{MILP}_{relax} \begin{cases} \underset{x,y,\eta}{\text{minimize}} & \eta \\ \text{subject to} & \eta \leq U^{k} - \varepsilon \\ & f(x^{k}, y^{k}) + \left(\nabla f(x^{k}, y^{k})\right)^{T} \begin{pmatrix} x - x^{k} \\ y - y^{k} \end{pmatrix} \leq \eta, \ \forall x^{k} \in \mathcal{X}^{k} \\ & g(x^{k}, y^{k}) + \left(\nabla g(x^{k}, y^{k})\right)^{T} \begin{pmatrix} x - x^{k} \\ y - y^{k} \end{pmatrix} \leq 0, \ \forall x^{k} \in \mathcal{X}^{k} \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^{p} \end{cases}$$

•  $\mathcal{X}^k \subset \mathcal{X} := \{ (\hat{x}^k, \hat{y}^k) \in X \times Y \cap \mathbb{Z}^p : (\hat{x}^k, \hat{y}^k) \text{ solutions to NLP}_{fix} \text{ or } NLP_{feas} \text{ for integer assignment } \hat{y} = y^k \}.$ 

- boundedness of  $Y \cap \mathbb{Z}^p \Longrightarrow$  boundedness of  $\mathcal{X}$  (and of  $\mathcal{X}^k$ ).
- upper bound  $U^k := \min_{j \le k} \{f(\hat{x}^k, \hat{y}^k) : \text{NLP}_{fix} \text{ is feasible} \}.$

## Outer Approximation: Pseudocode

**data**: starting integer point  $(x^0, y^0)$  and tolerance  $\varepsilon > 0$ . initialization: set  $U^{-1} := \infty$ ,  $\mathcal{X}^{-1} = \emptyset$  and k = 0.

#### repeat

Solve NLP<sub>fix</sub> or NLP<sub>feas</sub> with  $\hat{y} = y^k$ : solution  $(\hat{x}^k, \hat{y}^k)$ . **if** NLP<sub>fix</sub> is feasible and  $f(\hat{x}^k, \hat{y}^k) < U^{k-1}$  **then** Update best point  $(x^*, y^*) = (\hat{x}^k, \hat{y}^k)$  and  $U^k = f(\hat{x}^k, \hat{y}^k)$ .

else

Set  $U^{k} = U^{k-1}$ .

### end if

Add supporting hyperplanes about  $(\hat{x}^k, \hat{y}^k)$  to  $\mathsf{MILP}_{relax}$ :  $\mathcal{X}^k = \mathcal{X}^{k-1} \cup \{k\}.$ 

Solve MILP<sub>relax</sub>: solution  $(x^{k+1}, y^{k+1})$  and set k = k + 1. until MILP<sub>relax</sub> is infeasible.

## Worst case of OA [Hijazi et al., 2014]

**Theorem**. All previous assumptions hold. Then Outer Approximation terminates at optimal solution (or indication of infeasibility) of  $MINLP_{\eta}$  after a finite number of iterations.

$$P \begin{cases} \begin{array}{cc} \underset{y}{\text{minimize}} & 0\\ \text{subject to} & \sum_{i=1}^{p} \left(y_i - \frac{1}{2}\right)^2 \le \frac{p-1}{4}\\ & y \in \{0,1\}^p \end{cases}$$

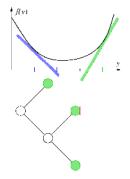
**Lemma**. Outer Approximation cannot cut more than one vertex of the hypercube:  $\text{MILP}_{relax}$  feasible for any  $k < 2^n$ .

**Corollary**. Outer Approximation Algorithm takes  $2^n$  iterations (each of them requires solving a MILP<sub>relax</sub>) to check infeasibility of nonlinear integer problem P.

# LP/NLP-based BB [Quesada and Grossman, 1992]

Aim: avoid solving expensive many MILP<sub>relax</sub>'s.

- Start solving MILP<sub>relax</sub> by Branch-and-Bound.
- If an integer solution  $(\tilde{x}, \tilde{y})$  is found  $\Rightarrow$  solve NLP<sub>fix</sub> with  $\hat{y} = \tilde{y}$ , get  $(\hat{x}, \hat{y})$ .
- Add supporting hyperplanes about  $(\hat{x}, \hat{y})$  to single Branch-and-Bound tree.
- Continue by solving MILP<sub>relax</sub> problem.
- Iterate until lower bound  $\geq$  upper bound.
- Never prune by integer feasibility.



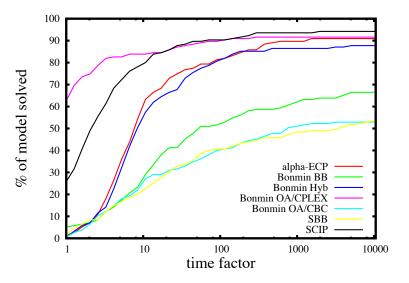


**Theorem.** All previous assumptions hold. Then LP/NLP-based Branchand-Bound terminates at optimal solution (or indication of infeasibility) of MINLP<sub> $\eta$ </sub> after a finite number of iterations.

# Convex MINLP Softwares [Bonami, 2014]

Solver	Reference	Algorithm(s)
Dicopt		OA
MINLP_BB	[Leyffer, 1998]	NLP BB
SBB	[Bussieck and Drud, 2001]	NLP BB
$\alpha$ -ECP	[Westerlund and Lundqvist, 2005]	ECP (variant of OA)
Bonmin	[Bonami et al., 2008]	NLP BB, OA, LP/NLP
Filmint	[Abhishek et al., 2010]	LP/NLP
KNITRO	[Byrd et al., 2006]	NLP BB, LP/NLP
SCIP	[Vigerske, 2013]	LP/NLP

## Convex MINLP Softwares [Bonami, 2014]



# Black Box MINLP: Derivative-free approaches

- objective function values are too expensive to compute.
- objective function values are determined via simulation.

### **Derivative-free methods:**

- Direct search: locally sampling objective function along a grid.
- Evolutionary methods: random mutations and survival of the fittest.

### Software:

• NOMAD (Nonsmooth Optimization by Mesh Adaptive Direct Search) [Audet et al., 2009], [Le Digabel, 2011].

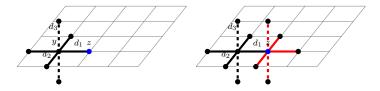


Figure: Local direct search [Liuzzi et al., 2014].

## Conclusions: Convex MINLP

• Extremely powerful and difficult: very challenging problem and many real-world applications.

• Convexity and completely knowledge of functions are critical assumptions.

• Key building blocks: NLP and MILP relaxations with constraint enforcement (branching and refinement).

• Basic algorithms for convex MINLP: Nonlinear Branch-and-Bound and Outer Approximation.

• One step beyond: LP/NLP-based Branch-and-Bound (Outer Approximation embedded in a single tree).

• MINLP softwares in a nutshell with a comparison picture: Outer Approximation performs relatively better.

• Reformulation is a very important ingredient in every optimization recipe: exploit structure of your problem.



Mathematical Programming, 74(2):121-140, 1996



### P. Bonami

#### Mixed Integer Nonlinear Programming Algorithms

Talk, 15ème Congrès Annuel de la Société Française de Recherche Opérationnelle et d'Aide à la Décision (ROADEF), Session Plénière, Université de Bordeaux. 2014



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An Exact Solution Approach for Integer Constrained Portfolio Optimization Problems Under Stochastic Constraints Operations Research, 57(3):650-670, 2009



P. Bonami, L.T. Biegler, A.R. Conn, G. Cornuéjols, I.E. Grossmann, C.D. Laird, J. Lee, A. Lodi, F. Margot, N. Sawaya and A. Wächter An Algorithmic Framework for Convex Mixed Integer Nonlinear Programs Discrete Optimization, 5(2):186-204, 2008



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Large-Scale Network Topological Optimization IEEE Transactions on Communications, 25(1):29-47, 1977

C. Bragalli, C. D'Ambrosio, J. Lee, A. Lodi and P. Toth On the Optimal Design of Water Distribution Networks: A Practical MINLP Approach Optimization and Engineering, 13(2):1-28, 2012



M.R. Bussieck and A. Drud

SBB: A New Solver for Mixed Integer Nonlinear Programming Talk, OR 2001, Section "Continuous Optimization", Duisburg, 2001



R.H. Byrd, J. Nocedal and R.A. Waltz

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