# 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

$$
\operatorname{MINLP} \begin{cases}\underset{x, y}{\operatorname{minimize}} & f(x, y) \\ \text { subject to } & g(x, y) \leq 0 \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^{p}\end{cases}
$$

- $f(x, y): \mathbb{R}^{n} \times \mathbb{R}^{p} \rightarrow \mathbb{R}, g(x, y): \mathbb{R}^{n} \times \mathbb{R}^{p} \rightarrow \mathbb{R}^{m}$ 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, robustness | number of assets, min investment |
| [Bienstock, 1996, Bonami and Lejeune, 2009, Vielma et al., 2008] |  |  |
| Chemical plant design | Chemical reactions | what to install |
| [Duran and Grossman | 1986, Flores-Tlacuah | and Biegler, 2007 |
| Block Layout Design [Castillo et al., 2005] | Spatial constraints | what to layout |
| Networks with delays | Delay as function of traffic | Path, flows |
| [Boorstyn and Frank, 1977, Ameur and Ouorou, 2006] |  |  |
| Location with stochastic services [Elhedhli, 2006] | Demands | location model |
| TSP with neighborhoods (Robotics) [Gentilini et al., 2013] | Definition of ngbh. | TSP |

## Real-world applications [Bonami, 2014]

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

## Convexity of Nonlinear Functions

$$
\operatorname{MINLP} \begin{cases}\underset{x, y}{\operatorname{minimize}} & f(x, y) \\ \text { subject to } & g(x, y) \leq 0 \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^{p}\end{cases}
$$

| Convex | Non-convex |
| :---: | :---: |
|  |  |

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

$$
f\left(x^{1}\right) \geq f\left(x^{0}\right)+\nabla f\left(x^{0}\right)^{T}\left(x^{1}-x^{0}\right)
$$

(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]).


## MINLP $\neq$ NLP

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

$$
\text { MILP } \begin{cases}\underset{x, y}{\operatorname{minimize}} & a^{T} x+b^{T} y \\ \text { subject to } & A x+B y \leq c \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^{p}\end{cases}
$$



- 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:

$$
\underset{y}{\operatorname{minimize}} \sum_{i=1}^{p}\left(y_{i}-\frac{1}{2}\right)^{2}, \quad \text { subject to } y_{i} \in\{0,1\}, \quad i=1, \ldots, p
$$

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



## Complexity Issues



- 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 $3 \Longrightarrow$ 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.


## Relax Integrality: NLP relax

$$
\text { NLP }_{\text {relax }} \begin{cases}\underset{x, y, \eta}{\operatorname{minimize}} & \eta \\ \text { subject to } & f(x, y) \leq \eta \\ & g(x, y) \leq 0 \\ & x \in X \\ & y \in Y\end{cases}
$$



- Relax integrality: from $y \in Y \cap \mathbb{Z}^{p}$ to $y \in Y \subset \mathbb{R}^{p}$.
- If MINLP $_{\eta}$ is convex then NLP $_{\text {relax }}$ is convex too (globally solvable).
- If $(\tilde{x}, \tilde{y})$ is optimal for NLP $_{\text {relax }}$ and feasible for MINLP $_{\eta}$, then it is also a minimum for MINLP $_{\eta}$.
- If $(\hat{x}, \hat{y})$ is feasible for $\operatorname{MINLP}_{\eta}$ and $f(\hat{x}, \hat{y})=f(\tilde{x}, \tilde{y})$, then it is also a minimum for MINLP $_{\eta}$.


## Relax Convex Nonlinearities: MILP ${ }_{\text {relax }}$

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

- Relax convex nonlinearities: supporting hyperplanes at points $\left(x^{k}, y^{k}\right)$ for $k \in K$ (apply the definition of nonlinear convex function).
- Polyhedral (linear) relaxation of nonlinear convex constraints.
- Same relationships between solutions of MILP relax and MINLP $P_{\eta}$.


## Relaxation in pictures



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

## Constraint Enforcement

$$
\operatorname{MINLP}_{\eta} \begin{cases}\underset{x}{\operatorname{minimize}} & \eta \\ \text { subject to } & f(x, y) \leq \eta \\ & g(x, y) \leq 0 \\ & x \in X \\ & y \in Y \cap \mathbb{Z}^{p}\end{cases}
$$



Goal: Exclude a solution ( $\tilde{x}, \tilde{y}$ ) of a relaxation, infeasible for of MINLP ${ }_{\eta}$.

- Relaxation refinement: tighten the MILP relax relaxation.
- Branching: exclude set of non-integer points from NLP relax.
- 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

$$
g_{j}(\tilde{x}, \tilde{y})+\nabla g_{j}(\tilde{x}, \tilde{y})^{T}\binom{x-\tilde{x}}{y-\tilde{y}} \leq 0
$$



Figure: $(\tilde{x}, \tilde{y})$ infeasible for MINLP $_{\eta}$ [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 $_{\text {relax }}$.

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

$$
y_{i} \leq\left\lfloor\tilde{y}_{i}\right\rfloor \quad \text { and } \quad y_{i} \leq\left\lceil\tilde{y}_{i}\right\rceil
$$

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


Figure: NLP subproblem with $y_{i} \leq\left\lfloor\tilde{y}_{i}\right\rfloor$ [Belotti et al., 2013].


Figure: NLP subproblem with $y_{i} \geq\left\lfloor\tilde{y}_{i}\right\rfloor$ [Belotti et al., 2013].

## Nonlinear Branch-and-Bound

$$
\text { NLP }_{\text {relax }} \begin{cases}\underset{x, y, \eta}{\operatorname{minimize}} & \eta \\ \text { subject to } & f(x, y) \leq \eta \\ & g(x, y) \leq 0 \\ & x \in X, y \in Y \\ & l \leq y \leq u\end{cases}
$$

$$
\left.\begin{array}{rl}
u^{+} & :=u \\
I^{+} & :=\left\lceil\tilde{y}_{i}\right\rceil
\end{array}\right\} \mathrm{NLP}_{\text {relax }}^{+}
$$

- solve NLP relax ${ }^{\text {and }}$ find a fractional solution $(\tilde{x}, \tilde{y})$.
- introduce two new sub-problems $\mathrm{NLP}_{\text {relax }}^{+}$and NLP $_{\text {relax }}^{-}$respectively with bounds $\left(I^{+}, u^{+}\right):=(I, u)$ and $\left(I^{-}, u^{-}\right):=(I, u)$ :

$$
u_{i}^{-}:=\left\lfloor\tilde{y}_{i}\right\rfloor \text { and } l_{i}^{+}:=\left\lceil\tilde{y}_{i}\right\rceil
$$

- nodes $\mathrm{NLP}_{\text {relax }}^{+}$and $\mathrm{NLP}_{\text {relax }}^{-}$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 ${ }_{\eta}$.
- 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 $f(\tilde{x}, \tilde{y}) \geq f(\hat{x}, \hat{y})$
$\Rightarrow$ no better integer solution in sub-tree.


## Nonlinear Branch-and-Bound: Pseudocode

initialization: set $U:=\infty$, and add NLP $_{\text {relax }}$ 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 $f(\tilde{x}, \tilde{y}) \geq U$ then
Prune node by dominance.
else if $(\tilde{x}, \tilde{y})$ is integral then
Update: $U:=f(\tilde{x}, \tilde{y})$ and $\left(x^{*}, y^{*}\right):=(\tilde{x}, \tilde{y})$.
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-andBound terminates at optimal solution (or indication of infeasibility) of MINLP $_{\eta}$ 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]

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

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


Figure: MILP ${ }_{\text {relax }}$ [Leyffer, 2013].

## Outer Approximation: NLP sub-problem

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

- NLP fix is feasible $\Longrightarrow$ upper bound to MINLP $_{\eta}$.
- NLP fix is infeasible $\Longleftrightarrow$ strictly positive optimal value of NLP $_{\text {feas }}$.
- NLP $_{\text {fix }}$ is infeasible $\Longrightarrow$ nonlinear solvers provide a solution to NLP $_{\text {feas }}$.

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

## Outer Approximation Algorithm

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

- $\mathcal{X}^{k} \subset \mathcal{X}:=\left\{\left(\hat{x}^{k}, \hat{y}^{k}\right) \in X \times Y \cap \mathbb{Z}^{p}:\left(\hat{\chi}^{k}, \hat{y}^{k}\right)\right.$ solutions to $\mathrm{NLP}_{\text {fix }}$ or NLP $_{\text {feas }}$ for integer assignment $\left.\hat{y}=y^{k}\right\}$.
- boundedness of $Y \cap \mathbb{Z}^{p} \Longrightarrow$ boundedness of $\mathcal{X}$ (and of $\mathcal{X}^{k}$ ).
- upper bound $U^{k}:=\min _{j \leq k}\left\{f\left(\hat{x}^{k}, \hat{y}^{k}\right): \operatorname{NLP}_{f i x}\right.$ is feasible $\}$.


## Outer Approximation: Pseudocode

data: starting integer point $\left(x^{0}, y^{0}\right)$ and tolerance $\varepsilon>0$.
initialization: set $U^{-1}:=\infty, \mathcal{X}^{-1}=\emptyset$ and $k=0$.
repeat
Solve NLP fix or NLP feas with $\hat{y}=y^{k}$ : solution $\left(\hat{x}^{k}, \hat{y}^{k}\right)$.
if $\operatorname{NLP}_{f i x}$ is feasible and $f\left(\hat{x}^{k}, \hat{y}^{k}\right)<U^{k-1}$ then
Update best point $\left(x^{*}, y^{*}\right)=\left(\hat{x}^{k}, \hat{y}^{k}\right)$ and $U^{k}=f\left(\hat{x}^{k}, \hat{y}^{k}\right)$.
else
Set $U^{k}=U^{k-1}$.
end if
Add supporting hyperplanes about $\left(\hat{x}^{k}, \hat{y}^{k}\right)$ to MILP relax : $\mathcal{X}^{k}=\mathcal{X}^{k-1} \cup\{k\}$.
Solve MILP relax : solution $\left(x^{k+1}, y^{k+1}\right)$ and set $k=k+1$.
until MILP ${ }_{\text {relax }}$ 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 $\eta_{\eta}$ after a finite number of iterations.

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



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

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

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

Aim: avoid solving expensive many MILP relax's.

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


Figure: LP/NLP-based BB [Leyffer, 2013].

Theorem. All previous assumptions hold. Then LP/NLP-based Branch-and-Bound terminates at optimal solution (or indication of infeasibility) of MINLP ${ }_{\eta}$ 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.


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