Solving Mixed-Integer Nonlinear Programs
(with SCIP)

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5th Porto Meeting on Mathematics for Industry, April 10–11, 2014, Porto

Outline

Solving MINLPs (with SCIP)

Solving convex MINLPs

Solving nonconvex MINLPs

Modeling, Reformulation, Presolving

Primal Solutions: The Undercover Heuristic

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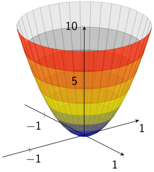
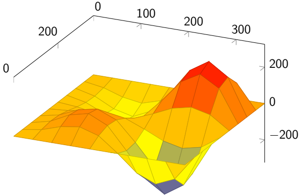
What is Mixed-Integer Nonlinear Programming?

$$
\begin{array}{lll}
\min & c^{\mathsf{T}} x & \text{for } c \in \mathbb{R}^n, \\
\text{s.t.} & \mathbf{g_k(x) \leqslant 0} & \text{for } k = 1, \dots, m,\ g_k : [\ell, u] \to \mathbb{R} \in C^1, \\
 & x \in [\ell, u], & \\
 & x_i \in \mathbb{Z} & \text{for } i \in \mathcal{I} \subseteq \{1, \dots, n\}.
\end{array}
$$



g_k **convex**

local = global optimality



g_k **nonconvex**

suboptimal local optima

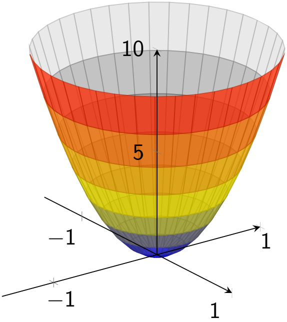
Convex MINLP

Assumption $g_1, \ldots, g_m$ convex

NLP-based

replace LP by NLP solver

branch on integer var.s with fractional NLP value



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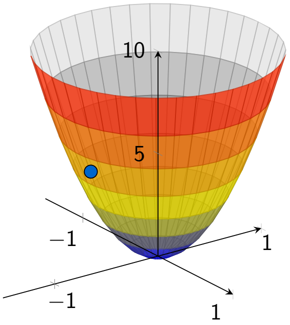

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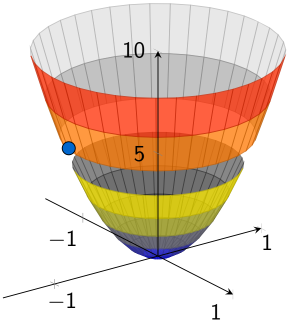

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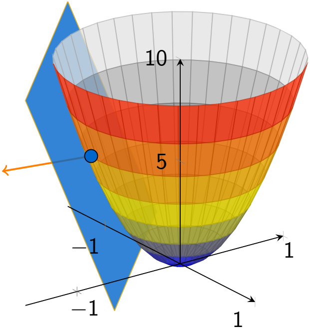
LP-based

underestimate by gradient cuts

$$g_k(\hat{x}) + \nabla g_k(\hat{x})^\mathsf{T}(x - \hat{x}) \leqslant 0$$



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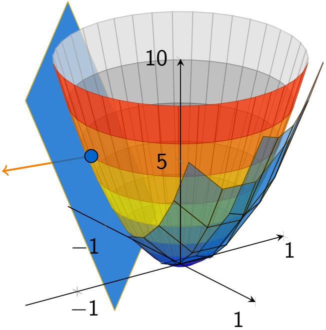
bound by polyhedral relaxation

- at MIP/NLP/sub-NLP solutions
- at node LP solutions



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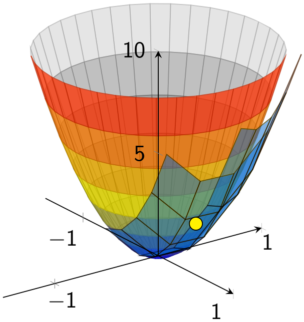

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Many algorithms, many solvers

α-ECP [Westerlund and Pettersson], BONMIN [Bonami et al.], DICOPT [Duran and Grossmann], sBB [ARKI Software & Consulting], ...

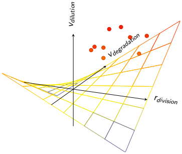
[see, e.g., Bonami, Biegler, Conn, Cornuéjols, Grossmann, Laird, Lee, Lodi, Margot, Sawaya, Wächter 2008]

Applications, applications, applications

- industrial engineering: mining with stockpiling constraints
- manufacturing: sheet metal design
- chemical industry: design of synthesis processes
- networks: operation and design of water and gas networks
- energy production and distribution: plant design, power scheduling
- biological engineering: cell modeling
- ...







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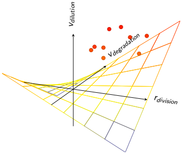

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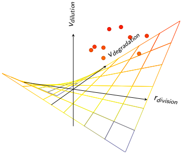

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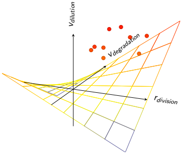

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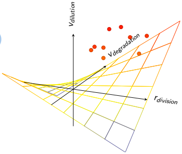

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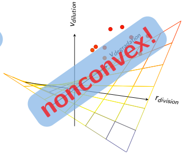
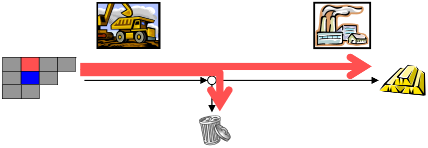




Variables:

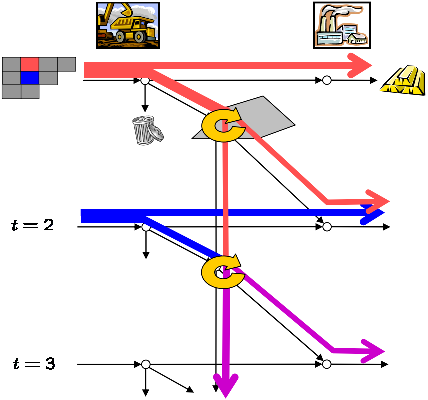
$x_{i,t} \in \{0,1\}$ block i fully mined by t

$f^{m}_{i,t} \in [0,1]$ % of block i mined in t

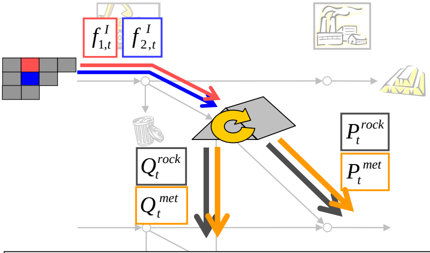
$f^{p}_{i,t} \in [0,1]$ % of block i processed in t

Constraints:

- material flow conservation
- mining & processing capacities
- mining precedences


$t = 2$
$t = 3$

Open Pit Mine Production Scheduling with Stockpiles



Aggregated stockpile model

$f^{I}_{i,t} \in [0,1]$ % of block i into stockpiled

Q_t^{rock}, Q_t^{met} total rock / metal tons held

P_t^{rock}, P_t^{met} total rock / metal tons out

Mixing constraints:

$$\frac{P_t^{met}}{Q_t^{met}} = \frac{P_t^{rock}}{Q_t^{rock}}$$ (metal fraction out = rock fraction out)

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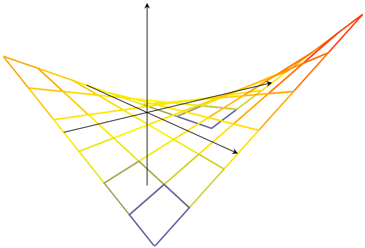

Relaxation

gradient cuts invalid

[McCormick 76, Smith and Pantelides 99, Tawarmalani and Sahinidis 02, Belotti et al. 09, Vigerske 13, ...]

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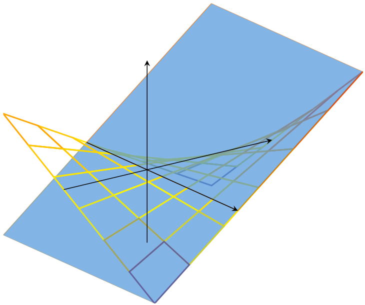

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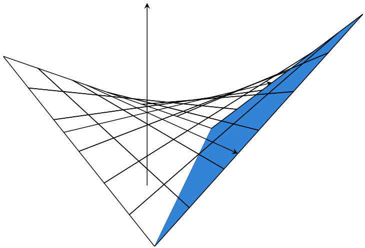

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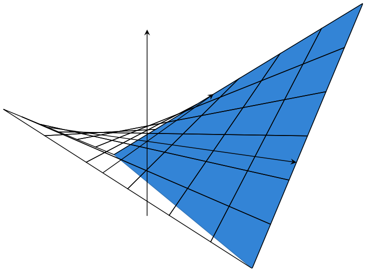

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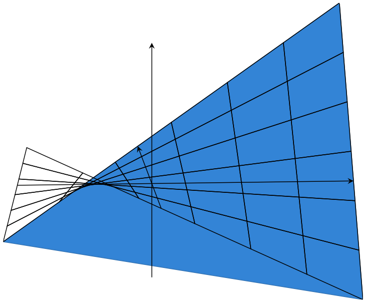

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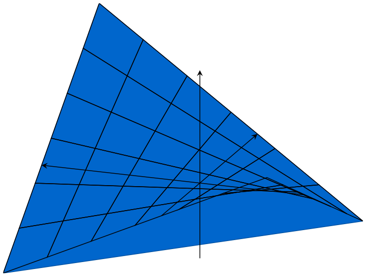

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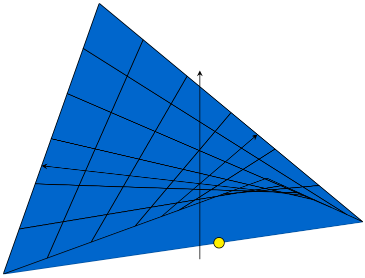

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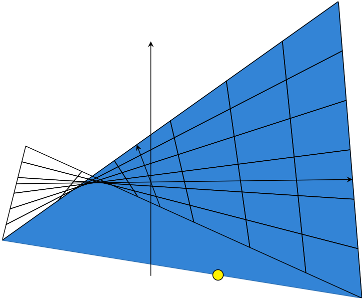

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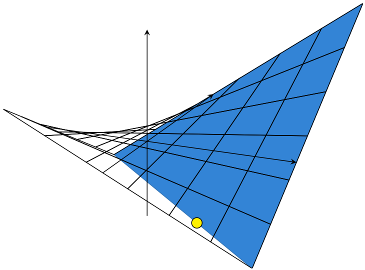

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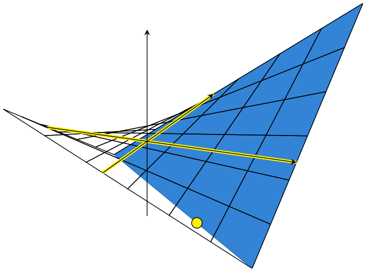

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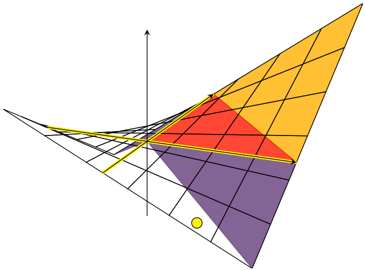

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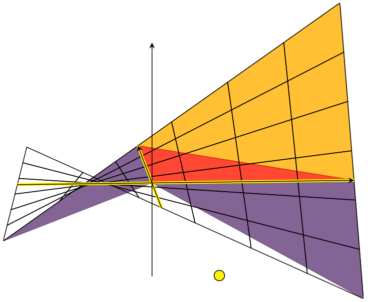

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Spatial branch-and-bound

branch on int. variables with fractional LP value

branch on variables in violated nonlinear constraints

[McCormick 76, Smith and Pantelides 99, Tawarmalani and Sahinidis 02, Belotti et al. 09, Vigerske 13, ...]

Convex Relaxation

Convex envelopes

- largest convex function that underestimates some $g_j(x)$
- difficult to find in general
- known for many elementary cases: convex, univariate concave, bilinear, ...

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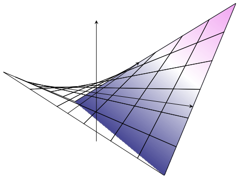
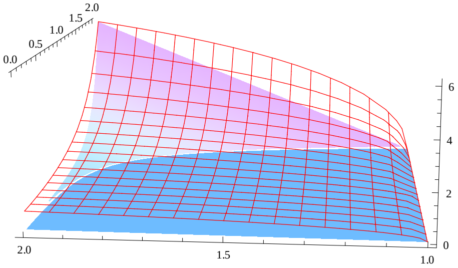


Convex Relaxation

Factorable functions

- recursive sum of products of univariate functions)
- reformulate into simple cases by introducing new variables and equations

$$g(x) = \sqrt{\exp(x_1^2)\ln(x_2)}$$
$$x_1 \in [0,2], \quad x_2 \in [1,2]$$



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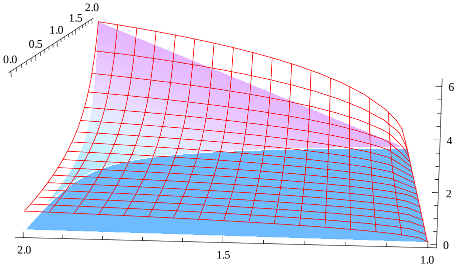

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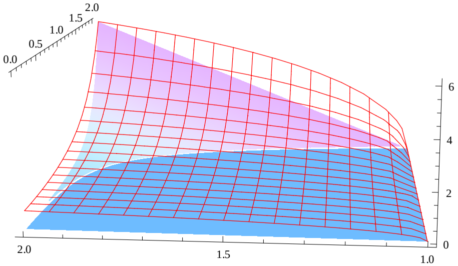
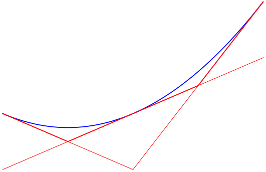


Tighter relaxations

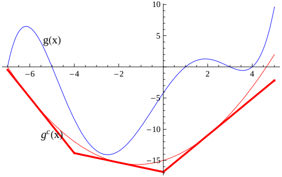
Reformulation-Linearization-Technique, SDP cuts, Disjunctive Programming, ...

General MINLP solving techniques

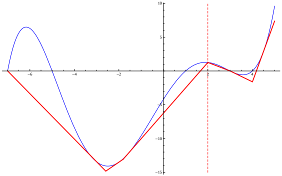
Gradient cuts



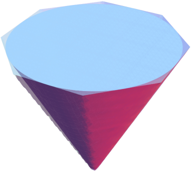
Underestimators



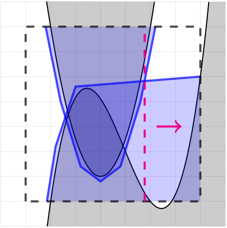
Spatial branching



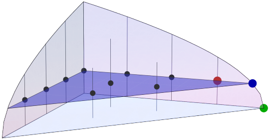
Presolving



Bound tightening



Primal heuristics



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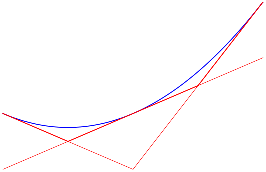

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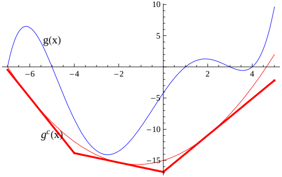

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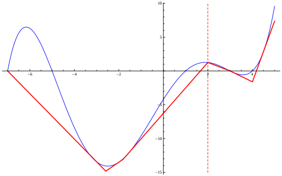
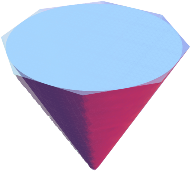
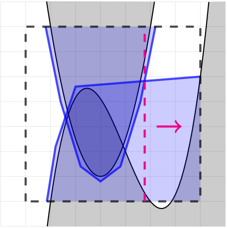


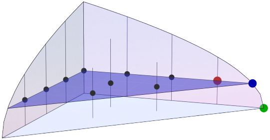
Presolving



Bound tightening



Primal heuristics



Outline

Solving MINLPs (with SCIP)

Modeling Considerations

Provide bounds on variables (as tight as possible)

- tighter relaxations

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- also intermediate expressions are important:

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$$\frac{x}{y} = 1 \qquad \Rightarrow \text{nonlinear and nonconvex}$$

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$$x = y \qquad \Rightarrow \text{linear and thus convex}$$

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$$xy \geqslant 1 \qquad \Rightarrow \text{nonconvex}$$

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Prefer Linearity and Convexity

$$y \geqslant \frac{1}{x} \qquad \Rightarrow \text{convex}$$

Reformulation of products with binary variables

A quadratic term

$$x \cdot \sum_{k=1}^{N} a_k y_k \quad \text{with} \quad x \in \{0,1\}$$

can be linearly reformulated:

- auxiliary continuous variable w
- additional linear constraints

$$M^L x \leqslant w \leqslant M^U x,$$

$$\sum_{k=1}^{N} a_k y_k - M^U(1-x) \leqslant w \leqslant \sum_{k=1}^{N} a_k y_k - M^L(1-x),$$

where M^L and M^U are bounds on $\sum_{k=1}^{N} a_k y_k$.

Convexity check for quadratic constraints

A quadratic constraint $x^\mathsf{T} A x + b^\mathsf{T} x \leqslant c$:

- convex if A is positive-semidefinite
- check by computing its minimal eigenvalue with `LAPACK`
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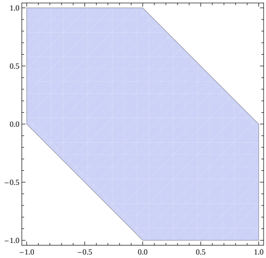

feasible region

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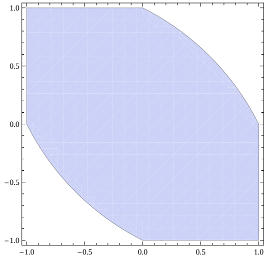

using McCormick underestimators:

$$\left\{ \begin{array}{c} x^2 + 2w + y^2 \leqslant 1 \\ w \geqslant L^y x + L^x y - L^x L^y \\ w \geqslant U^y x + U^x y - U^x U^y \end{array} \right\}$$

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A quadratic constraint $x^{\mathsf{T}}Ax + b^{\mathsf{T}}x \leqslant c$:

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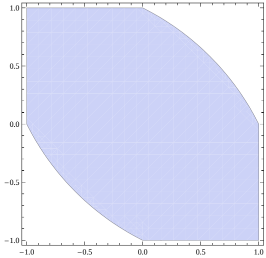

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branched into 4 subproblems

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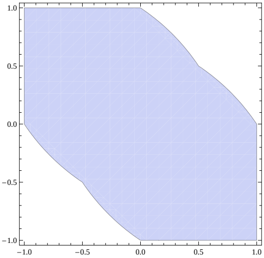

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branched into 16 subproblems

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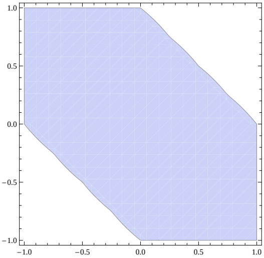

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branched into 64 subproblems

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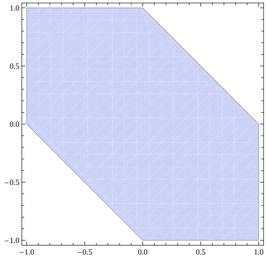


$$A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \text{ positive-semidefinite}$$

$\Rightarrow$ gradient cuts at 4 corners yield exact feasible region

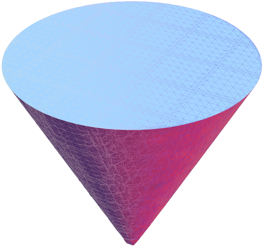
Second-order cone upgrade

Quadratic constraints of the form

$$\sum_{k=1}^{N} \alpha_k x_k^2 - \alpha_{N+1} x_{N+1}^2 \leqslant 0 \;\Leftrightarrow\; \sqrt{\sum_{k=1}^{N} \alpha_k x_k^2} \leqslant \sqrt{\alpha_{N+1}} x_{N+1}$$

with $\alpha_1, \ldots, \alpha_{N+1} \geqslant 0, L_{N+1} \geqslant 0$ describe a convex feasible region.

Example $x^2 + y^2 - z^2 \leqslant 0$ in $[-1, 1] \times [-1, 1] \times [0, 1]$



feasible region

"ice cream cone"

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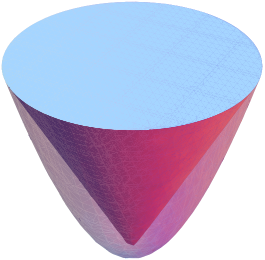

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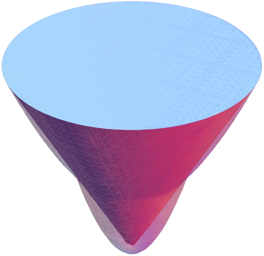

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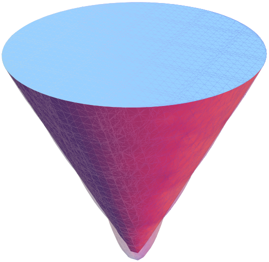

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after branching on $z = 0.25, 0.5, 0.75$

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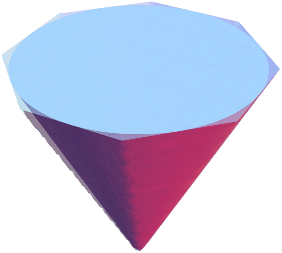
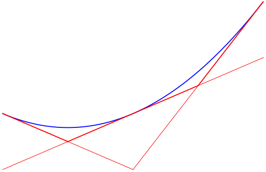


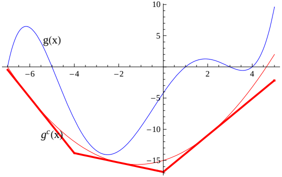
using gradient cuts at 8 corners

General MINLP solving techniques

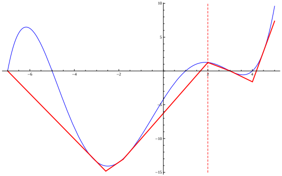
Gradient cuts



Underestimators



Spatial branching



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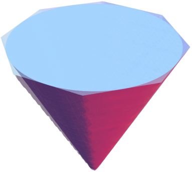

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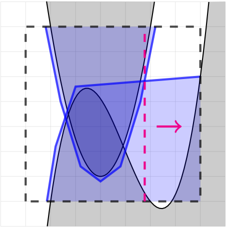

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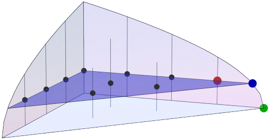

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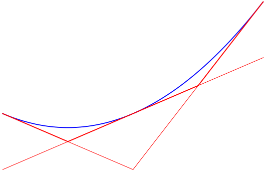

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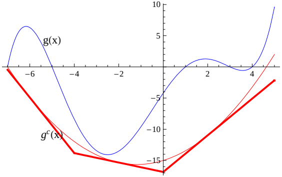

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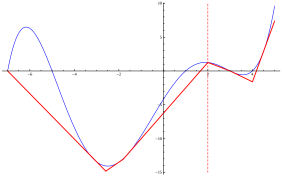

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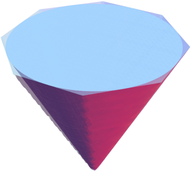

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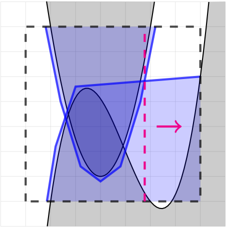

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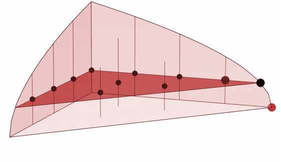


Solving MINLPs (with SCIP)

Primal Solutions

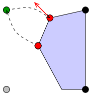
Feasible LP solutions . . .

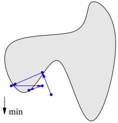
Standard MIP heuristics applied to MIP relaxation

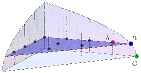
NLP local search

MINLP heuristics

- ▷ nonlinear feasibility pumps [Bonami et al. 2009, D'Ambrosio et al. 2010]
- ▷ RENS [Berthold 2013]
- ▷ Undercover [Berthold and G. 2013]







The Motivation

- Large Neighborhood Search: common paradigm in MIP heuristics

  fix a subset of variables $\rightsquigarrow$ easy subproblem $\rightsquigarrow$ solve

  MIP: "easy" = few integralities
  MINLP: "easy" = few nonlinearities

- observation: any MINLP can be reduced to a MIP by fixing (sufficiently many) variables.

  Experience: Often, few fixings are sufficient!

- idea: fix variables in minimum cover
- solution of LP/NLP relaxation as fixing values

The Structure

Definition Let us be given

- a domain box $[L, U] = \bigtimes_i [L_i, U_i]$,
- a function $g_j : [L, U] \to \mathbb{R}$, $x \mapsto g_j(x)$ on $[L, U]$, and
- a set $\mathcal{C} \subseteq \mathcal{N} := \{1, \ldots, n\}$ of variable indices.

We call $\mathcal{C}$ a cover of g if and only if for all $\bar{x} \in [L, U]$ the set

$$\{(x, g_j(x)) \mid x \in [L, U], x_k = \bar{x}_k \text{ for all } k \in \mathcal{C}\}$$

is an affine set intersected with $[L, U] \times \mathbb{R}$.

We call $\mathcal{C}$ a cover of P if and only if $\mathcal{C}$ is a cover for $g_1, \ldots, g_m$.

Covers of an MINLP

Definition Let P be an MINLP with $g_1, \ldots, g_m$ twice continuously differentiable on the interior of $[L, U]$.

We call $G_P = (V_P, E_P)$ the co-occurrence graph of P with

- node set $V_P = \{1, \ldots, n\}$ and
- edge set $E_P = \left\{ij \mid i, j \in V, \exists k \in \{1, \ldots, m\} : \frac{\partial^2}{\partial x_i \partial x_j} g_k(x) \not\equiv 0\right\}$,

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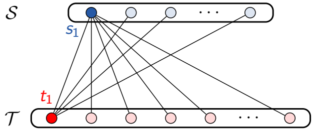
Example



$$\min \quad \dots \quad \text{s.t.} \quad s_1 t_i \leqslant a_i \text{ for all } i = 1, \dots$$
$$s_j t_1 \leqslant b_j \text{ for all } j = 1, \dots$$

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Theorem [Berthold and G. 2010, 2013]
$\mathcal{C} \subseteq \{1, \dots, n\}$ is a cover of P if and only if it is a vertex cover of the co-occurrence graph G_P.

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We call $G_P = (V_P, E_P)$ the co-occurrence graph of P with

- node set $V_P = \{1, \dots, n\}$ and
- edge set $E_P = \left\{ ij \mid i, j \in V, \exists k \in \{1, \dots, m\} : \frac{\partial^2}{\partial x_i \partial x_j} g_k(x) \not\equiv 0 \right\}$,

Theorem [Berthold and G. 2010, 2013]
$\mathcal{C} \subseteq \{1, \dots, n\}$ is a cover of P if and only if it is a vertex cover of the co-occurrence graph G_P.

Corollary Computing a minimum cover of an MINLP is $\mathcal{NP}$-hard.

Computing a minimum cover

Auxiliary binary variables

$$\alpha_k = 1 :\Leftrightarrow x_k \text{ is fixed in } P$$

$\mathcal{C}(\alpha) := \{k \mid \alpha_k = 1\}$ is a cover of P if and only if

$$\alpha_k = 1 \qquad \text{for all loops } kk \in E_P, \tag{1}$$

$$\alpha_k + \alpha_j \geqslant 1 \qquad \text{for all edges } kj \in E_p, k > j. \tag{2}$$

⇝ Covering problem

$$\min \Big\{ \sum_{k=1}^{n} \alpha_k : (1), (2), \alpha \in \{0,1\}^n \Big\}. \tag{3}$$

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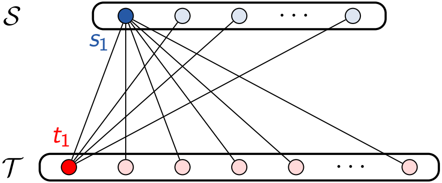
Optimization matters

The co-occurence graph of the bilinear program

$$\min \quad \dots \quad \text{s.t.} \quad s_1 t_i \leqslant a_i \text{ for all } i = 1, \dots,$$
$$s_j t_1 \leqslant b_j \text{ for all } j = 1, \dots,$$

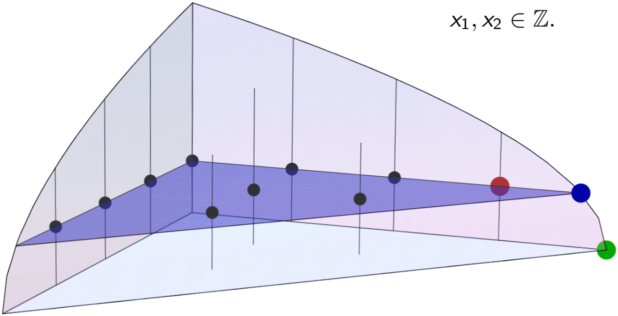
is



The cover $\mathcal{S}$ of complicating variables may be arbitrarily large compared to the minimum cover $\{s_1, t_1\}$.

A simple example

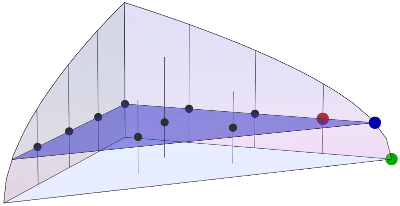
$$\begin{aligned} \max \quad & x_2 + x_3 \\ \text{s.t.} \quad & x_1 + x_2 + x_3^2 \leqslant 4, \\ & x_1, x_2, x_3 \geqslant 0, \\ & x_1, x_2 \in \mathbb{Z}. \end{aligned}$$



Fixing x_3 to any value within its bounds yields a linear subproblem.

The Undercover Heuristic

Input: MINLP P
begin
compute a solution $\bar{x}$ of an approximation of P;
round $\bar{x}_k$ for all $k \in \mathcal{I}$;
determine a cover $\mathcal{C}$ of P;
solve the sub-MIP of P given by fixing $x_k = \bar{x}_k$ for all $k \in \mathcal{C}$;



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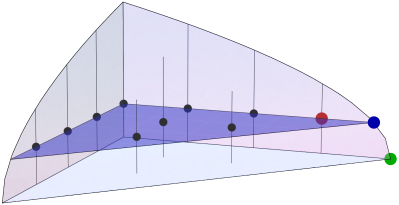

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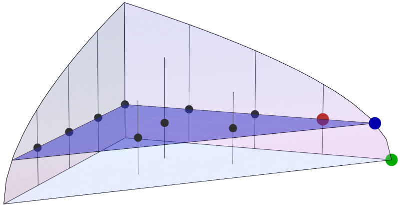

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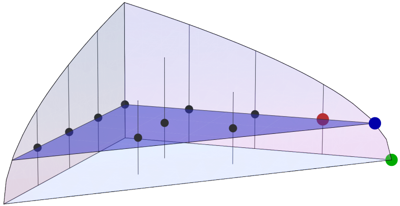

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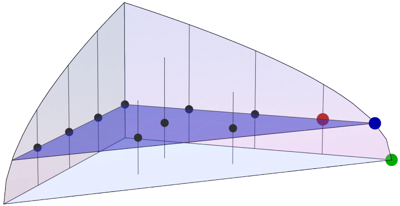

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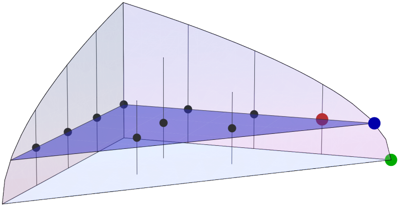


Remark:

- MIP heuristics: trade-off fixing many vs. few variables

  here: eliminate nonlinearities by fixing as few as possible variables

  $\rightarrow$ minimum cover!

NLP postprocessing

NLP postprocessing

- All sub-MIP solutions are fully feasible for the original MINLP.
- Still, sub-MIP solution $\tilde{x}$ could be improved by NLP local search:
  - fix all integer variables of the original MINLP to their values in $\tilde{x}$
  - solve the resulting NLP to local optimality

Fix-and-propagate & Backtracking

Fix-and-propagate

- Do not fix variables in $\mathcal{C}$ simultaneously, but sequentially and propagate after each fixing.
- If $x_k^\star$ falls out of bounds then
  - fix to the closest bound (similar to [FischettiSalvagnin09])
  - recompute the approximation

Backtracking

- If fix-and-propagate deduces infeasibility, apply a one-level backtracking: undo last fixing and try another value

Avoiding/exploiting Infeasibility

If the sub-MIP is infeasible, this is typically detected

- during fix-and-propagate, or
- via infeasible root LP.

$\rightsquigarrow$ Generate conflict clauses for the original MINLP

- Add them to the original MINLP.
- Use them to revise fixing values and/or fixing order
- Start another fix-and-propagate run

If the sub-MIP remains infeasible, at least this gives us valid conflicts to prune the search tree in the original problem.

Computational experiments

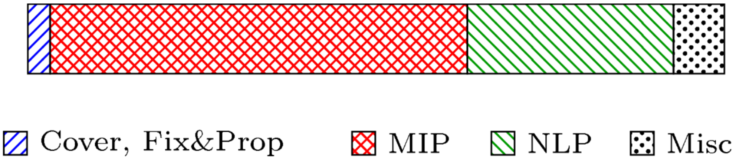
Test set

- 149 MIQCPs from GloMIQO test set

Comparison to other heuristics

- Undercover: solution for 76 instances (typically less than 0.1 sec)
- root heuristics: Baron 65, Couenne 55, SCIP 98
- lower success rate on general MINLPs

Undercover components



Take-away messages

- SCIP can solve nonconvex MINLPs to global optimality
- like other solvers: Antigone/GloMIQO, BARON, Couenne, ...

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- convex modelling/reformulation/detection crucial
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Thank you very much for your attention!

Muito obrigado!

Solving Mixed-Integer Nonlinear Programs
(with SCIP)

Ambros M. Gleixner

Zuse Institute Berlin · Matheon · Berlin Mathematical School

5th Porto Meeting on Mathematics for Industry, April 10–11, 2014, Porto