# LP/MIP based techniques for solving MINLPs

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**DFG Research Center MATHEON**
**Mathematics for key technologies**

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# Overview

1. Convex MINLP
   - Algorithms
   - Extensions
   - Solvers
2. Nonconvex MINLP
   - Spatial Branch-and-Bound Algorithm
   - Solvers
   - Application: Mine Production Scheduling
   - Techniques

## Mixed Integer Nonlinear Program (MINLP)

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\begin{aligned}
\text{minimize} \quad & f(x) \\
\text{such that} \quad & g_j(x) \leq 0, \qquad j \in J, \\
& x \in X = \{x \in \mathbb{R}^n : Dx \leq d, \underline{x} \leq x \leq \overline{x}\}, \\
& x_I \in \mathbb{Z}^{|I|},
\end{aligned}
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where

- $f : X \to \mathbb{R}$ and $g_j : X \to \mathbb{R}$, $j \in J$, are differentiable functions
- $I \subseteq \{1, \ldots, n\}$ the set of integer variables

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Important Special Cases:

- Convex MINLP: $f$ and $g_j$ are convex functions on $X$
- MIQQP (Mixed Integer Quadratically Constraint Quadratic Program): $f$ and $g_j$ are quadratic functions

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Survey papers:

- I.E. Grossmann, Review of Nonlinear Mixed-Integer and Disjunctive Programming Techniques, 2002
- P. Bonami, M. Kilinç, J. Linderoth, Algorithms and Software for Convex Mixed Integer Nonlinear Programs, 2010

# Outline

Some NLP subproblems that will be useful:

## NLP relaxation

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### Feasibility subproblem

$$\begin{aligned} \min\ & u \\ \text{s.t. } & g_j(x) \leq u,\ j \in J, \\ & x \in X, \quad u \in \mathbb{R}, \\ & x_I = \hat{x}_I \end{aligned}$$

- $\hat{x}_I \in X_I \cap \mathbb{Z}^{|I|}$ a candidate for integer part of a solution
- solution yields minimal infeasible solution w.r.t. $\hat{x}_I$

- replace nonlinearities in MINLP by supporting hyperplanes (use convexity)
- given $K$ points $x^k$, $k = 1, \ldots, K$

## MIP outer-approximation of MINLP

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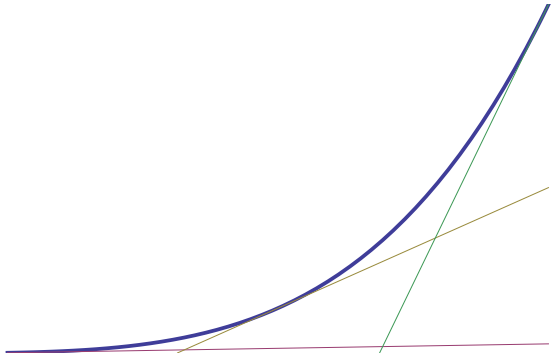
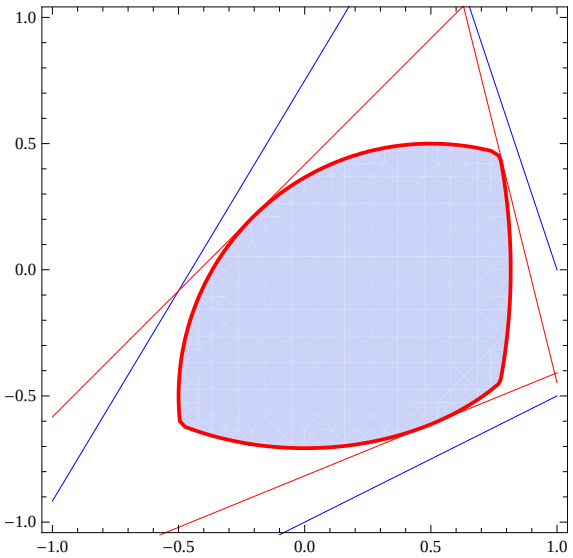
\begin{aligned}
\min\ & \alpha \\
\text{s.t. } & \alpha \geq f(x^k) + \nabla f(x^k)^T (x - x^k), \qquad k=1,\ldots,K, \\
& g_j(x^k) + \nabla g_j(x^k)^T (x - x^k) \leq 0, \qquad j \in J^k,\ k=1,\ldots,K, \\
& x \in X, \quad x_I \in \mathbb{Z}^{|I|}
\end{aligned}
$$

with $J^k \subseteq J$ set of constraints for which to include linearization in $x^k$



underestimate objective




overestimate feasible region

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  - branch on fractional integer variables
  - performs well if NLP relaxation is tight
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  - similar to Outer-Approximation
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- LP/NLP-based Branch-and-Bound [Quesada and Grossmann, 1992, Bonami et al., 2008, Abhishek et al., 2010]

# Outer-Approximation for Convex MINLP

[Duran and Grossmann, 1986, Yuan et al., 1988, Fletcher and Leyffer, 1994]

## Basic Theorem [Duran and Grossmann, 1986]

MINLP and the following problem have the same optimal solution

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Idea: relax equivalent MIP to MIP approximation by solving a sequence of NLP sub- and feasibility problems

## Outer-Approximation Algorithm [Duran and Grossmann, 1986]

1. solve NLP relaxation
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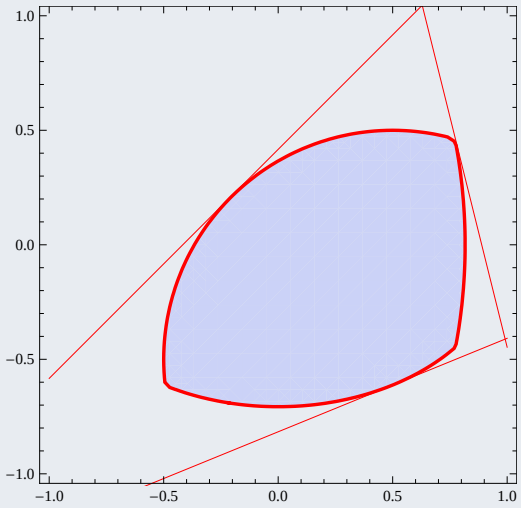

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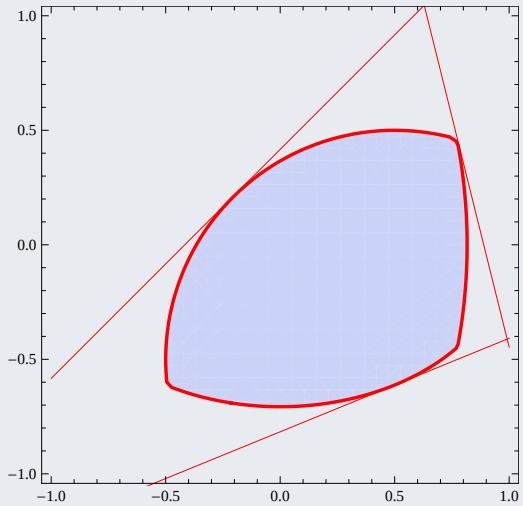

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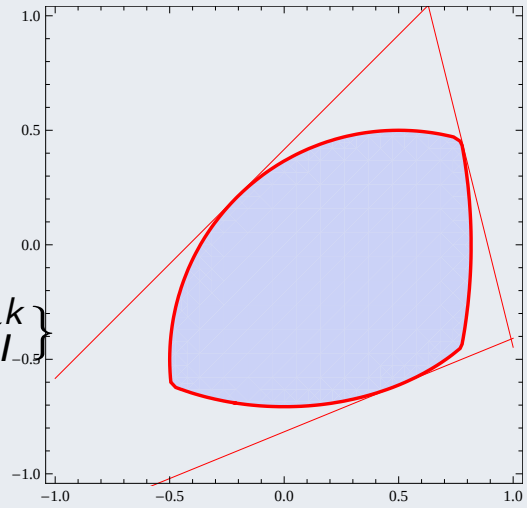

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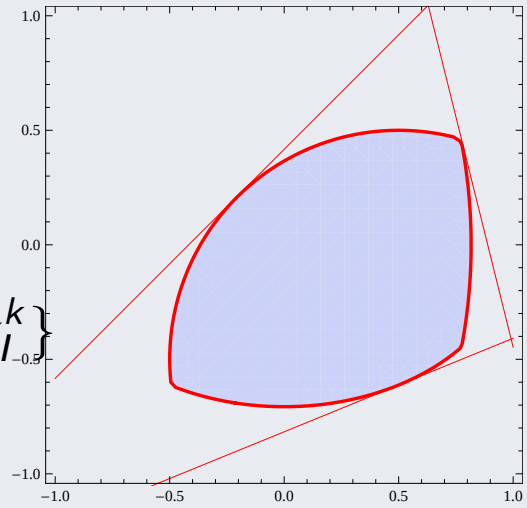

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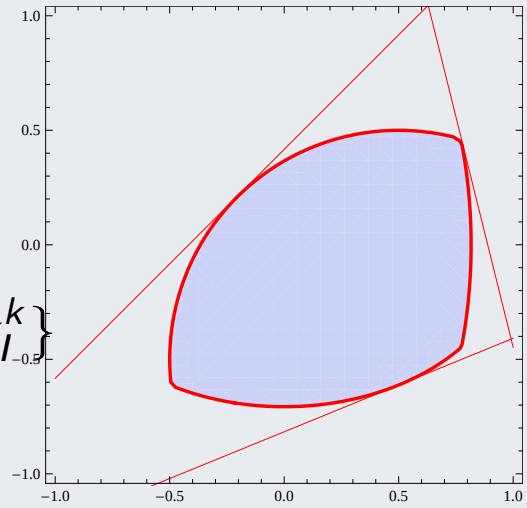
   - 3.5 add linearizations of $g_j(\cdot)$ in $x^k$ to MIP relaxation
   - 3.6 optional: if $X_I \subseteq [0,1]^{|I|}$, add cut to forbid $x_I^k$ in MIP



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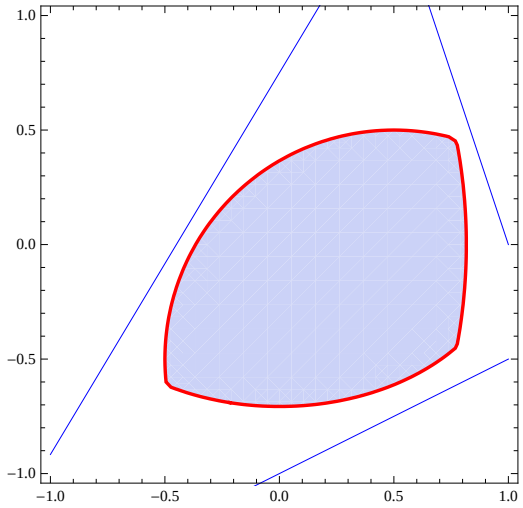

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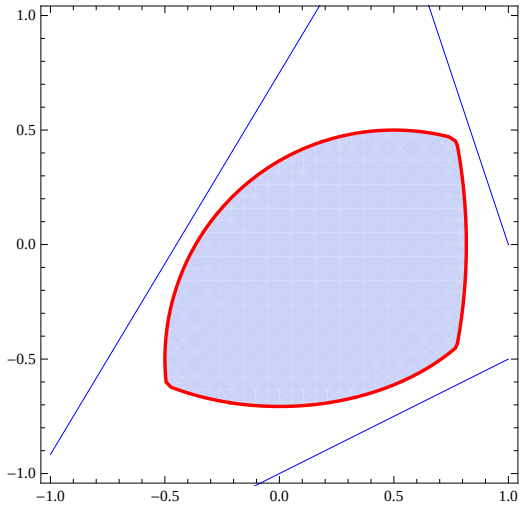

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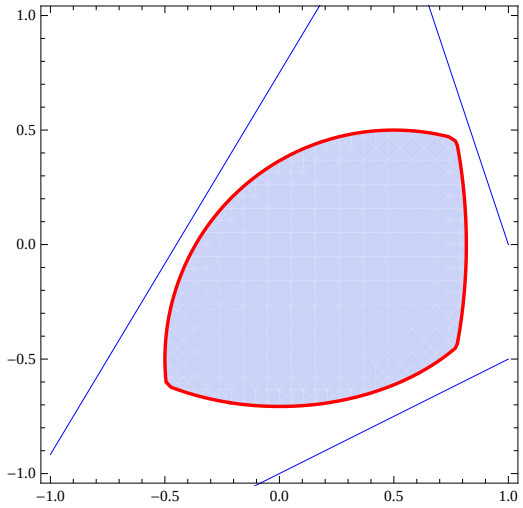

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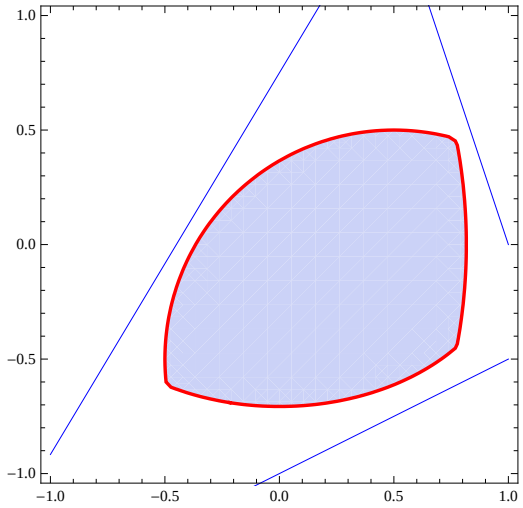


- works well on almost linear problems

# LP/NLP based Branch-and-Bound

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$$\text{or} \quad x^k := \text{argmin}\{u : g_j(x) \leq u,\ j \in J,\ \ x \in X,\ \ u \in \mathbb{R},\ \ x_I = \tilde{x}^k_I\}$$

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- proposed relaxation [Kocis and Grossmann, 1987]:

$$\begin{aligned} \nabla h_j(x^k)^T(x - x^k) &\leq 0, \qquad \text{if } \lambda_j^k > 0, \\ \nabla h_j(x^k)^T(x - x^k) &\geq 0, \qquad \text{if } \lambda_j^k < 0, \end{aligned}$$

  where $\lambda_j^k$ is the dual multiplier associated with $h_j(x, y) = 0$ in the NLP, $j \in J_=$

- remains a rigorous method only in special cases

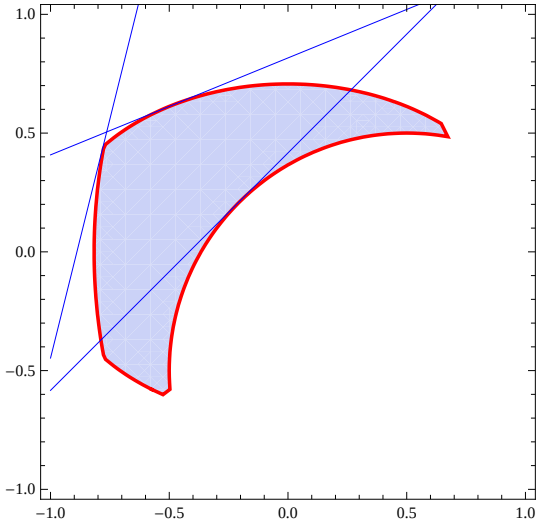
# Reducing Effect of Nonconvexity

Assume $f(\cdot)$ or $g_j(\cdot)$ nonconvex or nonlinear equalities $h(x, y) = 0$ present.

$\Rightarrow$ Outer-Approximation runs in two difficulties:

1. NLP subproblems may not be solved to global optimality
2. gradient-based linearizations may cut into feasible region

$\Rightarrow$ apply heuristic strategies to reduce effect of nonconvexity



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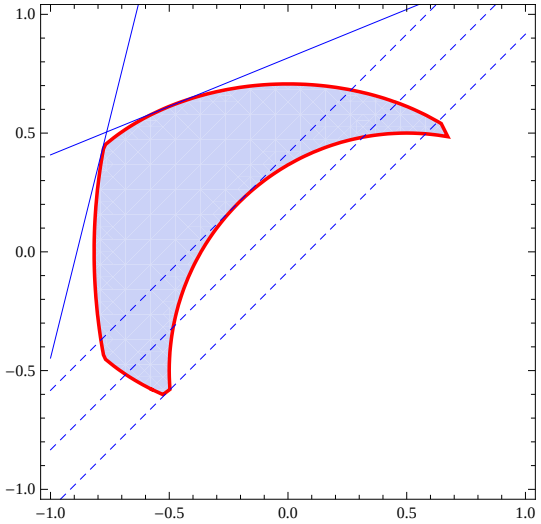


## Augmented Penalty / Equality Relaxation MIP master problem

[Viswanathan and Grossmann, 1990]

$$
\begin{aligned}
\min\ & \alpha + \sum_{k=1}^{K} w_p^k p^k + w_q^k q^k \\
\text{s.t. } & \alpha \geq f(x^k) + \nabla f(x^k)^T (x - x^k), && k = 1, \ldots, K, \\
& g_j(x^k) + \nabla g_j(x^k)^T (x - x^k) \leq p^k, && j \in J, k = 1, \ldots, K, \\
& \text{sign}(\lambda_k) \nabla h_j(x^k)^T (x - x^k) \leq q^k, && j \in J_=, k = 1, \ldots, K, \\
& x \in X, \quad x_I \in \mathbb{Z}^{|I|}, \quad \alpha \in \mathbb{R}, \quad p^k, q^k \geq 0
\end{aligned}
$$

# Branching and Node Selection Strategies

Consider LP/NLP based Branch-and-Bound.

Similar Strategies as in MIP:

- pseudo-cost branching
- strong branching
- reliability branching

- depth first search
- best first search
- diving methods
- two-phase methods

# Cutting Planes

Consider LP/NLP based Branch-and-Bound.

Cutting Planes for convex MINLP:

- ▷ MIP cutting planes (Gomory, MIR, flowcover, ...)

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- Gomory Cuts for conic constraints [Cezik and Iyengar, 2005]
- Mixed Integer Rounding for Second-Order-Cone Constraints: [Atamtürk and Narayanan, 2010]

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- Mixed Integer Rounding for Second-Order-Cone Constraints: [Atamtürk and Narayanan, 2010]
- disjunctive inequalities / lift-and-project: [Stubbs and Mehrotra, 1999, Drewes, 2009, Kilinç et al., 2010a]
- simple lift-and-project inequality from (strong) branching: [Kilinç et al., 2010b]

$$\alpha \geq \hat{\alpha}_i^- + (\hat{\alpha}_i^+ - \hat{\alpha}_i^-)x_i,$$

where $\hat{\alpha}_i^-$ = lower bound for $x_i = 0$; $\hat{\alpha}_i^+$ = lower bound for $x_i = 1$
20% improvement in mean solve time for FilMINT [Bonami et al., 2010]

Heuristics for MINLP:

- diving heuristics for NLP-based branch-and-bound [Bonami and Gonçalves, 2008]
  - as in MIP, but try to fix several variables at each iteration
  - dive such that all nonlinear integer variables get integral values, then fix all nonlinear variables (to current value in NLP relaxation), solve remaining MIP
  - 21% improvement in mean B&B time

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# The Feasibility Pump for MINLP

[Bonami et al., 2009a, Bonami and Gonçalves, 2008]

Basic Idea: Create a sequence of integer feasible points $\hat{x}^k$ and nonlinear feasible points $x^k$ by alternating solution of

## MIP relaxation

$$\begin{aligned} \hat{x}^{K+1} := \text{argmin } & \|x - x^K\|_1 \\ \text{s.t. } & g_j(x^k) + \nabla g_j(x^k)^T(x - \bar{x}^k) \leq 0, \quad j \in J, \quad k \leq K \\ & x \in X, \qquad x_I \in \mathbb{Z}^{|I|} \end{aligned}$$

## NLP relaxation

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## Alternative: Rounding

$$\hat{x}^{K+1} := \text{argmin } \|x - x^K\|_1$$

s.t.

$$x_I \in \mathbb{Z}^{|I|}$$

## NLP relaxation

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s.t. $g_j(x) \leq 0, \quad j \in J$

$$x \in X$$

- Convergence for convex problems: finds feasible point $x^K$ or proofs infeasibility
- Heuristic for nonconvex problems
- Rounding variant finds solution for 93% of the instances;
  2.7% improvement in mean branch-and-bound time
  [Bonami and Gonçalves, 2008]

Perspective Relaxation: [Günlük et al., 2007, Hijazi et al., 2009, Günlük and Linderoth, 2010]
Disjunctive Programming: [Grossmann and Lee, 2003, Vecchietti and Grossmann, 1999]

# Outline

# Solvers that implement NLP based Branch–and–Bound

**SBB = Simple Branch and Bound** [GAMS Development Corp., 2010]

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[Bonami et al., 2008]

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- uses CBC, CPLEX for MIP and IPOPT, FilterSQP for NLP
- option B-BB = NLP-based Branch-and-Bound
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## MINLP_BB = Mixed Integer NonLinear Programming Branch&Bound

[Leyffer, 2001]

- developed by S. Leyffer
- based on FilterSQP and bqpd
- advanced (strong) branching and node selection techniques

# Solvers that implement Outer Approximation Algorithm

## DICOPT = Discrete and Continuous Optimizer

[Viswanathan and Grossmann, 1990]

- developed by J. Viswanathan and I.E. Grossmann (CMU)
- available within GAMS only
- implements augmented penalty / equation relaxation approach to cope with nonconvexities and equalities

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# Solvers implementing Extended Cutting Plane Alg.

## AlphaECP = $\alpha$ Extended Cutting Plane [Westerlund and Pörn, 2002]

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- experimental

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**FilMINT = Filter-Mixed INTeger optimizer** [Abhishek et al., 2010]

- developed by K. Abhishek, J.T. Linderoth (Lehigh), and S. Leyffer (Argonne)
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- option B-QG = Quesada-Grossmann LP/NLP-based Branch-and-Bound
- option B-Hyb = alternate between LP and NLP relaxation in nodes
- implemented as extension of CBC

# Solvers implementing LP/NLP-based Branch&Bound

## KNITRO

[Byrd et al., 2006]

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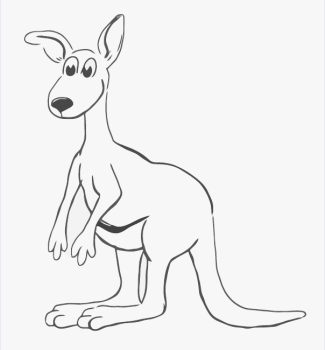
## SCIP = Solving Constraint Integer Programs

[Achterberg, 2007, Berthold et al., 2009a]

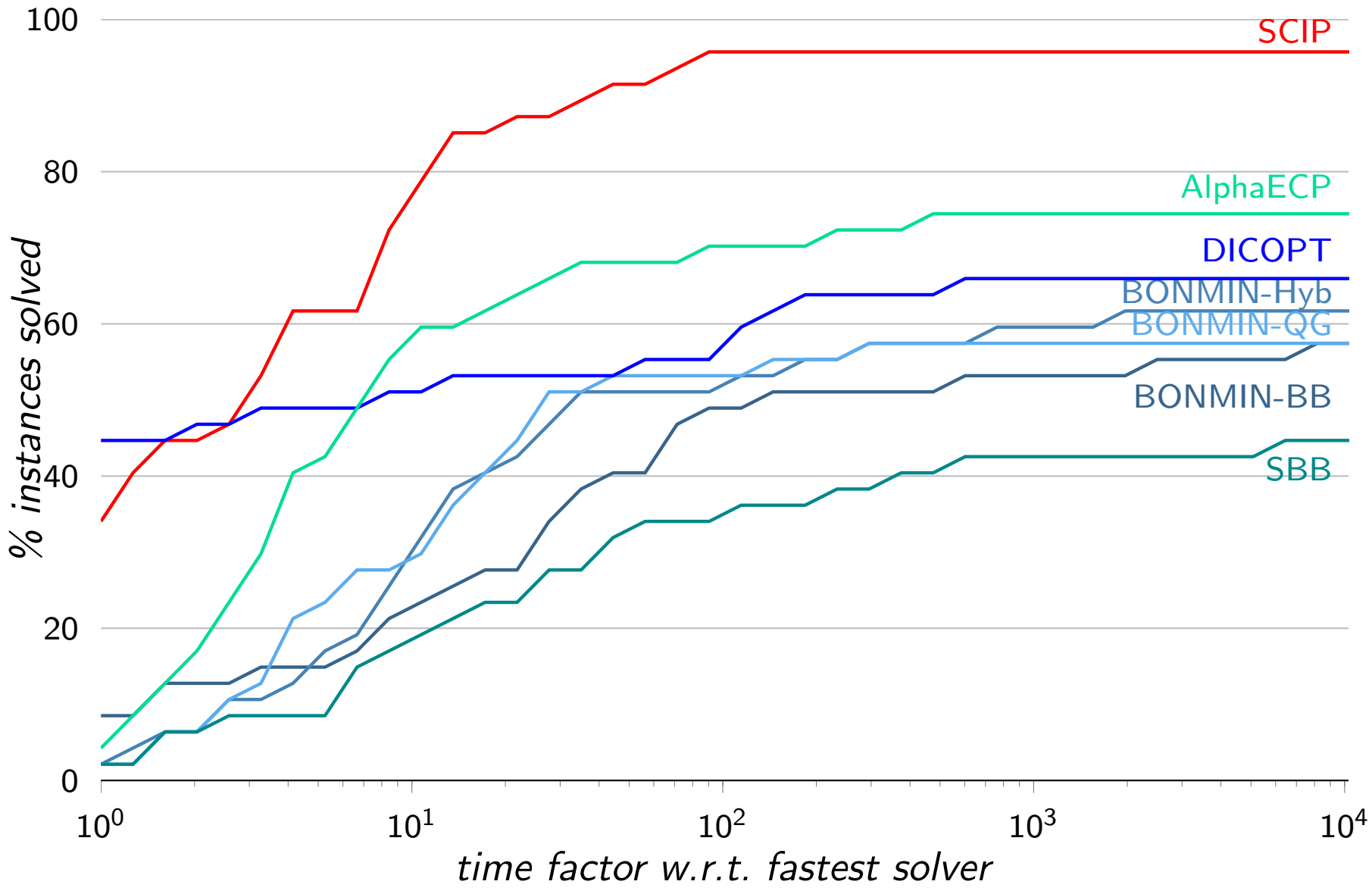
- since 1.2.0: support for MIQQP
- general MINLP in development
- close to extended cutting plane



Experimental Environment:

- test set from [Bonami et al., 2009b]: 48 convex MINLP instances from various applications
- solvers:
  - AlphaECP 1.75.04
    CPLEX for MIPs and CONOPT for NLPs
    option `ECPstrategy 1`
  - BONMIN 1.3 in variants B-BB, B-QG, and B-Hyb
    CBC for MIPs and IPOPT for NLPs
  - DICOPT 2x-C
    CPLEX for MIPs and CONOPT for NLPs
    options `stop 1`, `maxcycles 10000`
  - SBB
    CONOPT for NLPs
    option `memnodes 9999999`
  - SCIP 1.2.0.7 with experimental support for convex nonlinear constraints
    CPLEX for LPs and IPOPT for NLPs
- timelimit 1 hour, gap tolerance $10^{-4}$
- 2.5GHz Intel Core2 Duo, 4GB RAM

# Benchmark on 48 convex MINLPs



# Overview: Nonconvex MINLP

1. Convex MINLP
   - Algorithms
   - Extensions
   - Solvers
2. Nonconvex MINLP
   - Spatial Branch-and-Bound Algorithm
   - Solvers
   - Application: Mine Production Scheduling
   - Techniques

Some key papers:

- M. Tawarmalani and N. Sahinidis, Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications, 2002
- P. Belotti, J. Lee, L. Liberti, F. Margot, and A. Wächter, Branching and bounds tightening techniques for non-convex MINLP, 2009

# Outline

# How to solve Nonconvex MINLPs?

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{such that} \quad & g_j(x) \leq 0, \qquad j \in J \\ & x \in X, \\ & x_I \in \mathbb{Z}^{|I|} \end{aligned}$$

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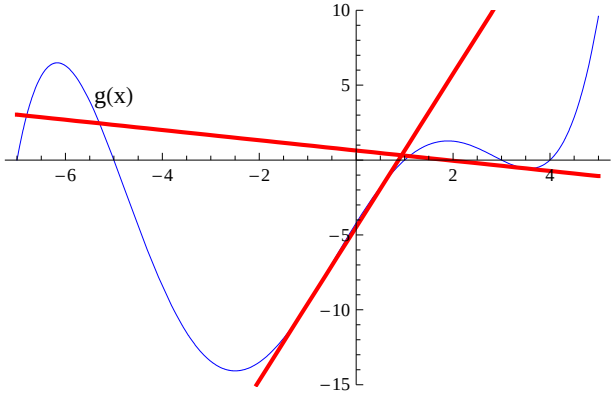
$\Rightarrow$ inequalities $g_j(\hat{x}) + \nabla g_j(\hat{x})^T (x - \hat{x}) \leq 0$ may not be valid!



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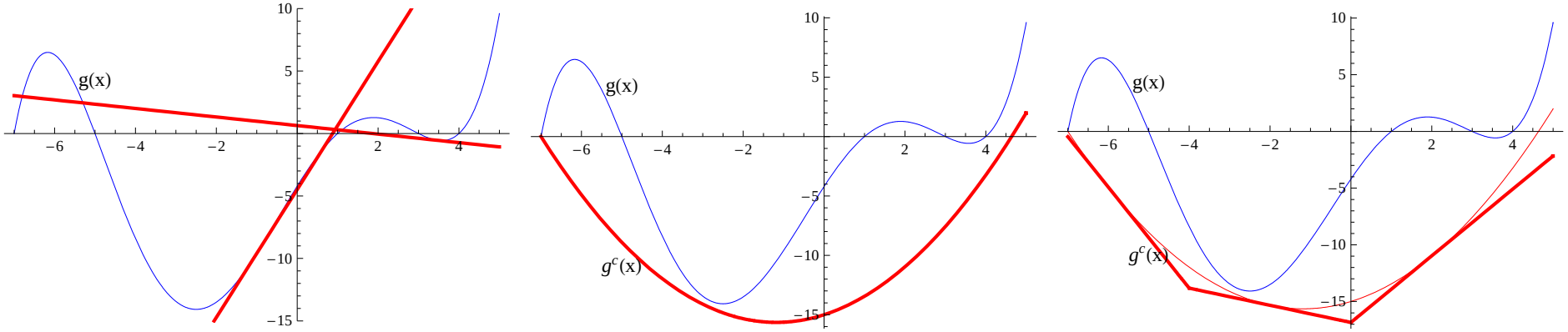
$\Rightarrow$ use techniques from global optimization of NLPs

$\Rightarrow$ use convex underestimator: convex and below $g(x)$ for all $x \in X$

$\Rightarrow$ introduces convexification gap



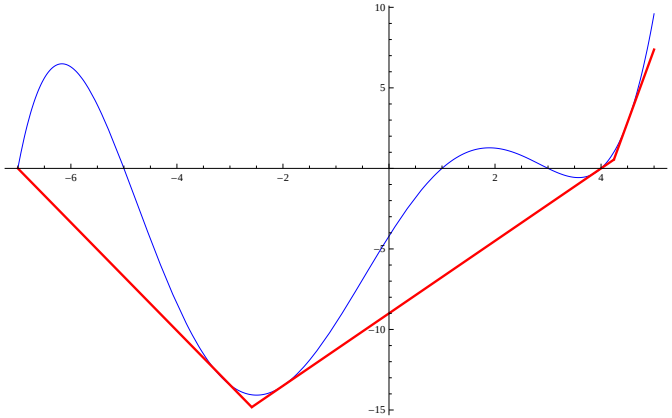
# Spatial branch-and-bound Algorithm

[Smith and Pantelides, 1999, Tawarmalani and Sahinidis, 2002]

In each node with local bounds $[\underline{x}, \overline{x}]$:

Bounding: generate a linear outer-approximation w.r.t. $[\underline{x}, \overline{x}]$ using convexification and linearization techniques

$$\begin{aligned} \min \quad & \alpha \\ \text{s.t.} \quad & Ax + A'\alpha \leq b, \\ & x \in X, \quad x \in [\underline{x}, \overline{x}] \end{aligned}$$



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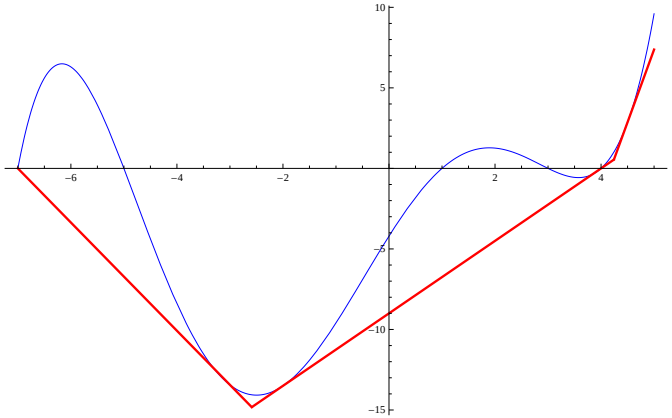
Branching: close gap between relaxation and problem

- ▷ branch on integer variables with fractional value in LP



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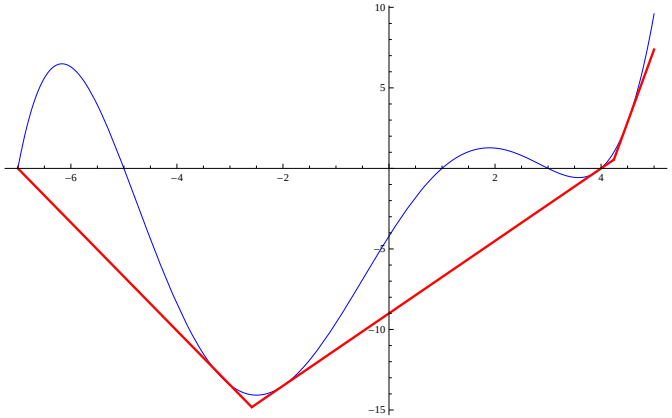
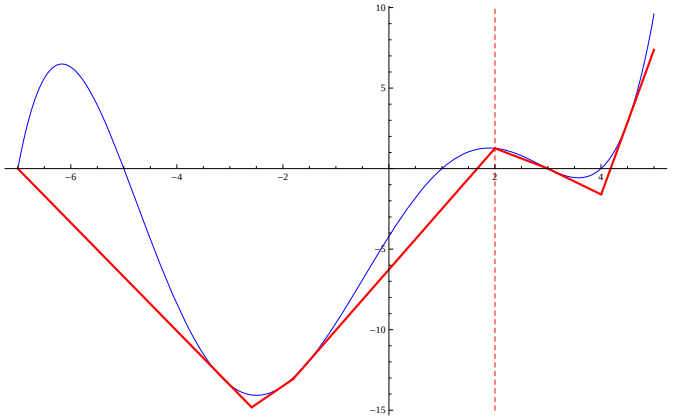
- ▷ branch on continuous variables in nonconvex terms

  $\Rightarrow$ smaller domain $\Rightarrow$ tighter relaxation





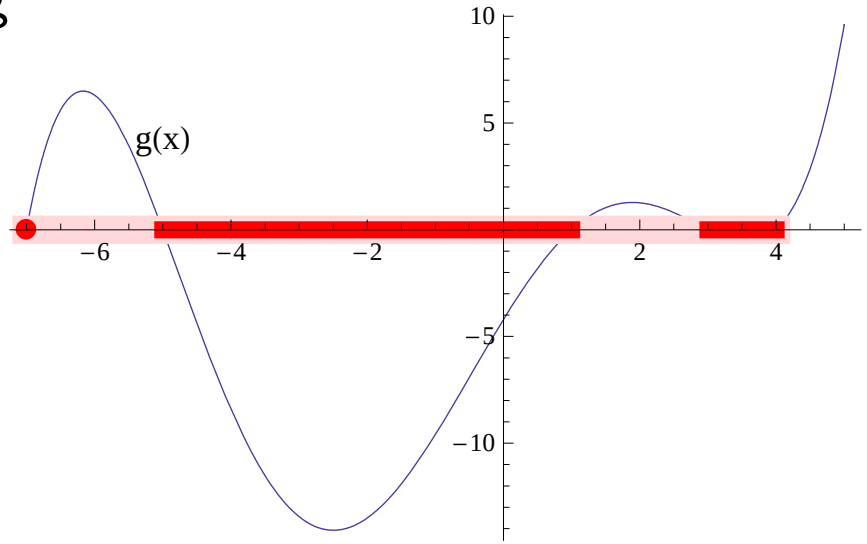
# The linear outer-approximation of a nonconvex MINLP

Given: A function $g : \mathbb{R}^n \to \mathbb{R}$ defining the constraint

$$g(x) \leq 0, \qquad x \in [\underline{x}, \overline{x}]$$

Seek: A (linear) outer-approximation of

$$\mathrm{conv}\{x \in [\underline{x}, \overline{x}] : g(x) \leq 0\}$$



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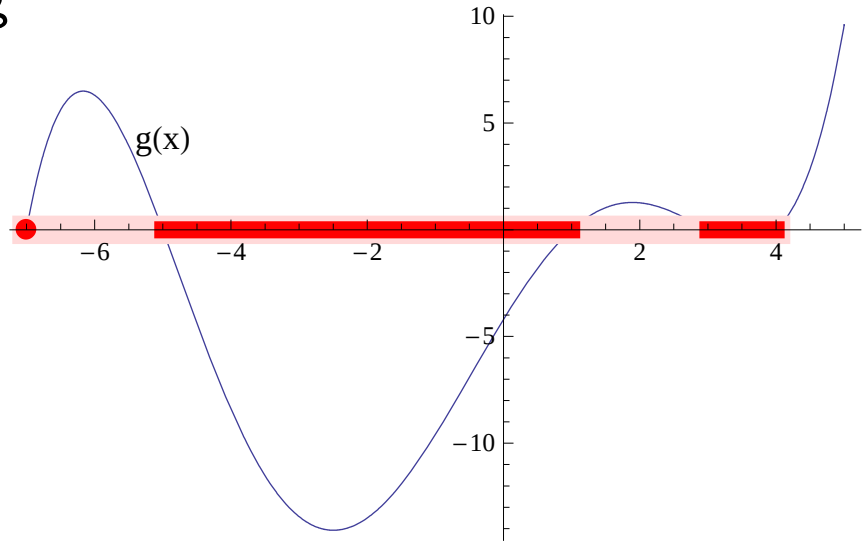


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$\Rightarrow$ too difficult in general

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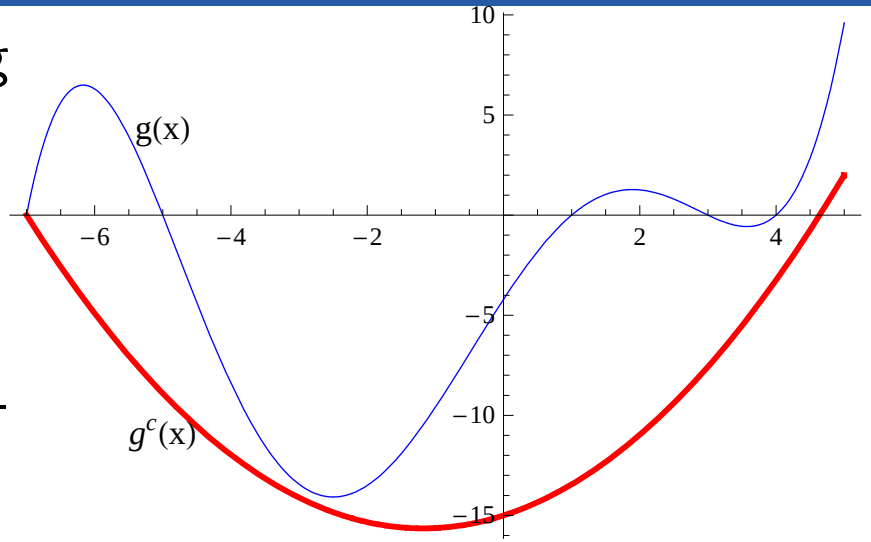
Seek: A convex function $g^c(\cdot)$ that underestimates $g(\cdot)$ on $[\underline{x}, \overline{x}]$:




$$\{x \in [\underline{x}, \overline{x}] : g(x) \leq 0\} \subseteq \{x \in [\underline{x}, \overline{x}] : g^c(x) \leq 0\}$$

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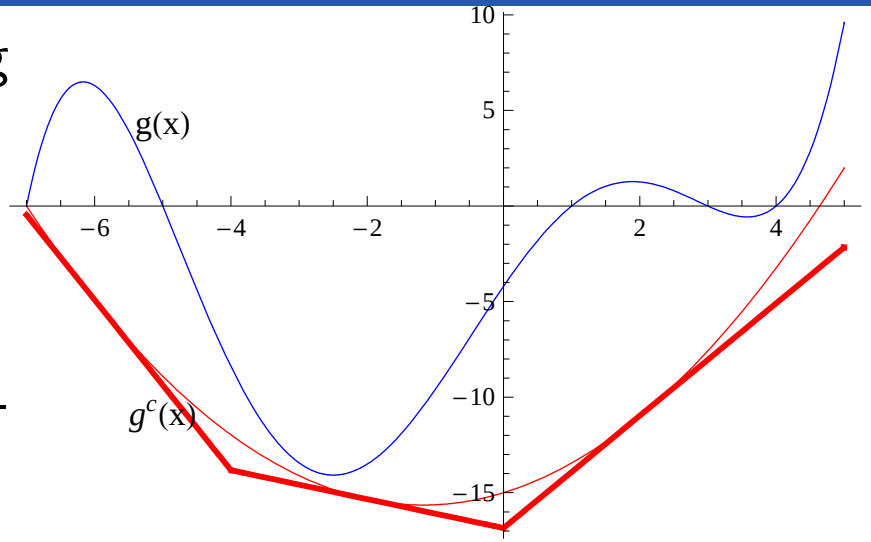


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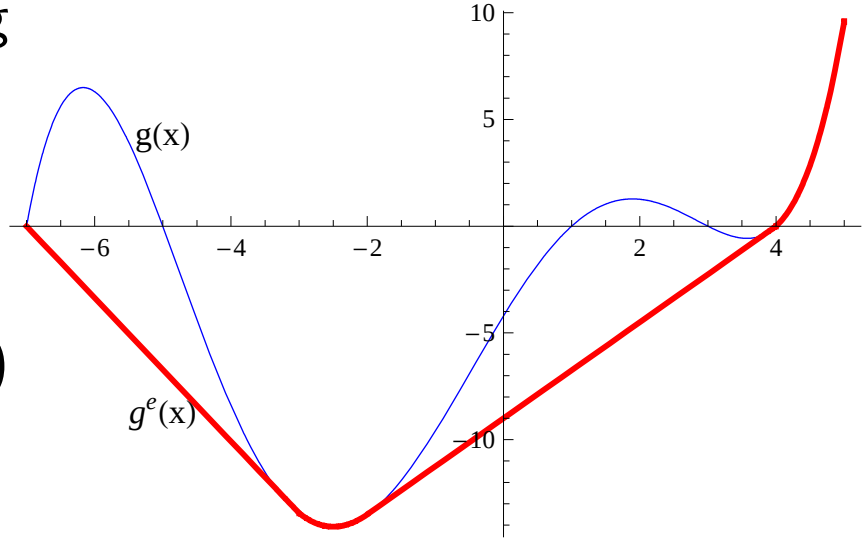



Seek: The tightest convex function $g^c(\cdot)$ that underestimates $g(\cdot)$ on $[\underline{x}, \overline{x}]$:

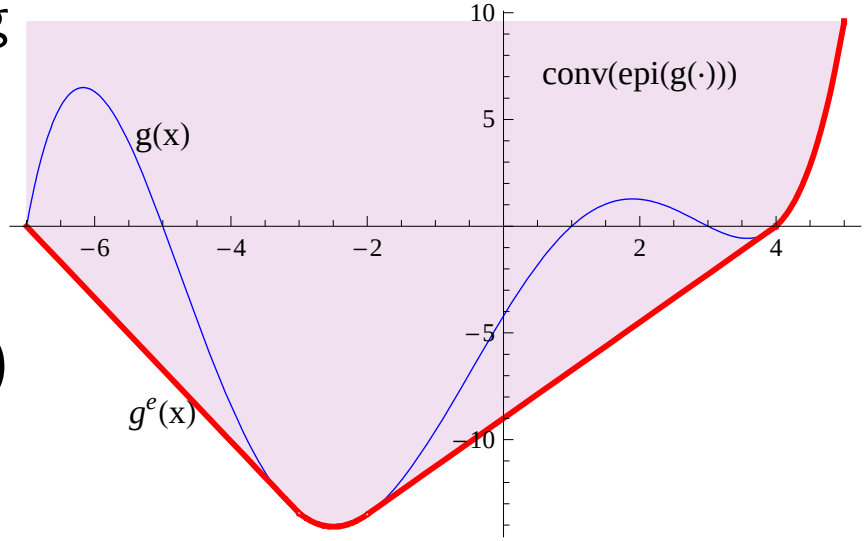
The convex envelope $g^e : [\underline{x}, \overline{x}] \to \mathbb{R}$ is a function such that

- ▷ analytically:
  - $g^e(x)$ is convex on $[\underline{x}, \overline{x}]$
  - $g^e(x) \leq g(x)$ for all $x \in [\underline{x}, \overline{x}]$
  - $\forall h : [\underline{x}, \overline{x}] \to \mathbb{R}$, $h(\cdot)$ convex, $h(\cdot) \leq g(\cdot)$: $h(\cdot) \leq g^e(\cdot)$

# The linear outer-approximation of a nonconvex MINLP

Given: A function $g : \mathbb{R}^n \to \mathbb{R}$ defining the constraint

$$g(x) \leq 0, \qquad x \in [\underline{x}, \overline{x}]$$




Seek: The tightest convex function $g^c(\cdot)$ that underestimates $g(\cdot)$ on $[\underline{x}, \overline{x}]$:

The convex envelope $g^e : [\underline{x}, \overline{x}] \to \mathbb{R}$ is a function such that

- ▷ analytically:
  - $g^e(x)$ is convex on $[\underline{x}, \overline{x}]$
  - $g^e(x) \leq g(x)$ for all $x \in [\underline{x}, \overline{x}]$
  - $\forall h : [\underline{x}, \overline{x}] \to \mathbb{R}$, $h(\cdot)$ convex, $h(\cdot) \leq g(\cdot)$: $h(\cdot) \leq g^e(\cdot)$
- ▷ geometrically: $\mathrm{epi}(g^e(\cdot)) = \mathrm{conv}(\mathrm{epi}(g(\cdot)))$

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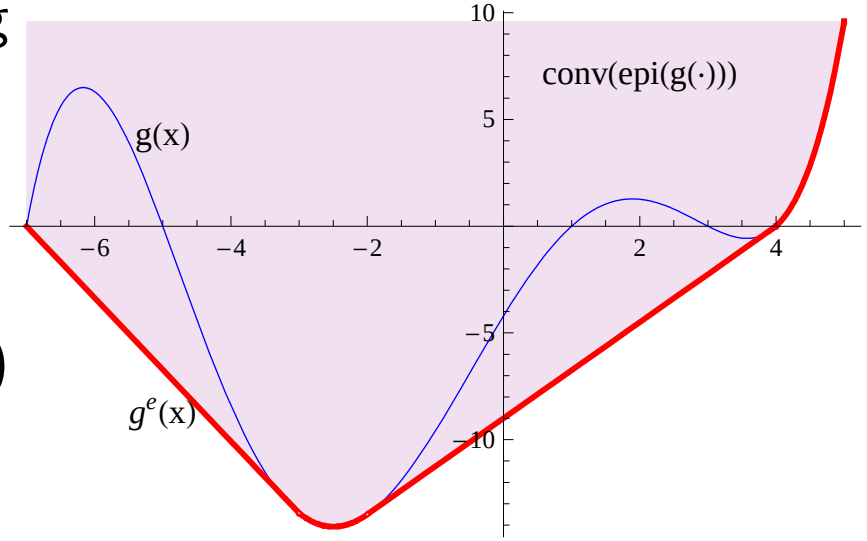


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In general: Convex envelopes are hard to find.

(finding the convex envelope of a function is as hard as finding its global min.)

# Convex envelopes for concave functions

# Convex envelopes for concave functions

**Theorem (Tawarmalani and Sahinidis [2002])**

*Let $v_1, \ldots, v_k$ be the vertices of a polytope $P$. The convex envelope $g^e(x)$ of a concave function $g(x)$ over $P$ can be expressed as*

$$g^e(x) = \min_{\alpha} \sum_{i=1}^{k} \lambda_i g(v_i)$$

$$\text{s.t.}\, x = \sum_{i=1}^{k} \lambda_i v_i, \qquad \sum_{i=1}^{k} \lambda_i = 1, \qquad \lambda_i \geq 0, \quad i = 1, \ldots, k$$

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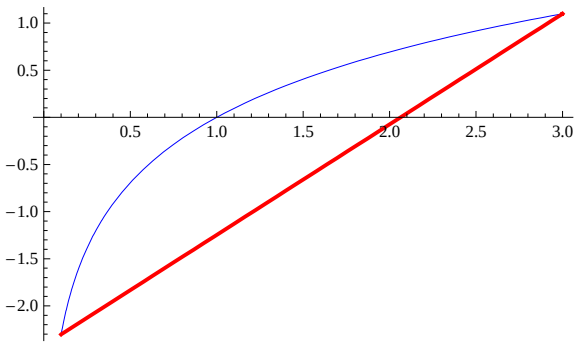
- For now: Special case $n = 1$, $P = [\underline{x}, \overline{x}]$
- Convex envelope for univariate concave functions is the secant between $\underline{x}$ and $\overline{x}$.
  $\Rightarrow \log(x), -\exp(x), -x^{2k}, \sqrt{x}, \ldots$



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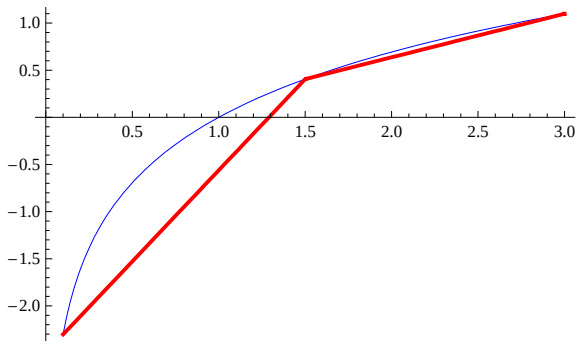
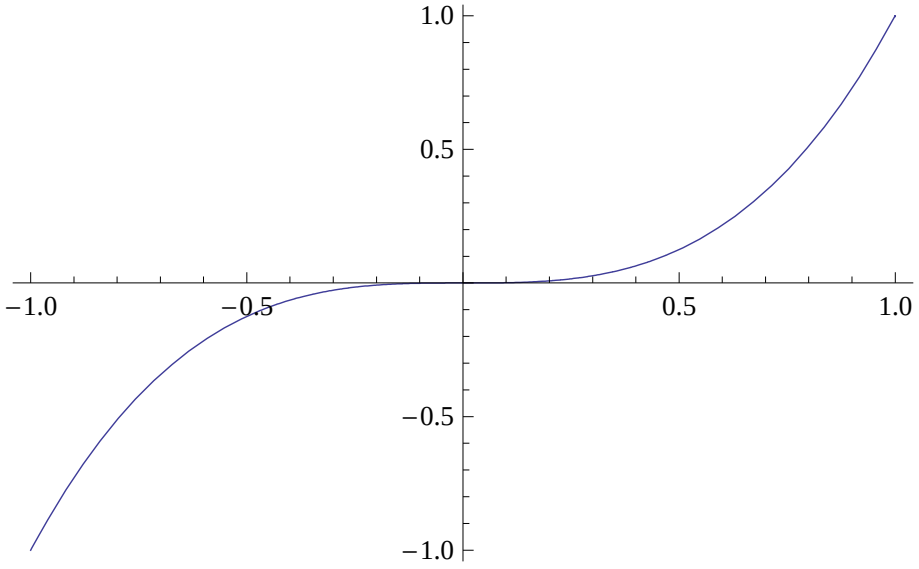
- In branch-and-bound: tighten by branching



# Convex envelope for monomials of odd degree

[Liberti and Pantelides, 2003]

$$g(x) = x^{2k+1}, \qquad k \in \mathbb{N}$$



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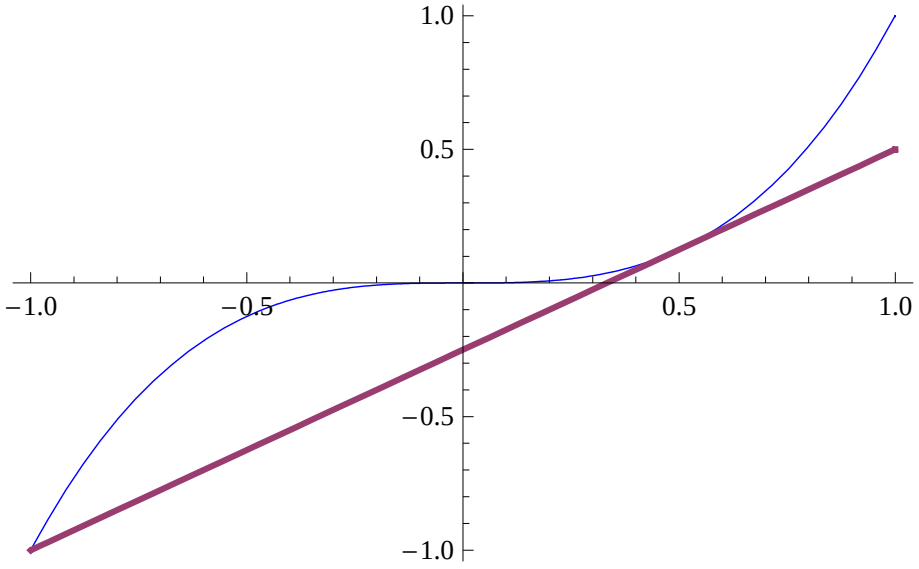

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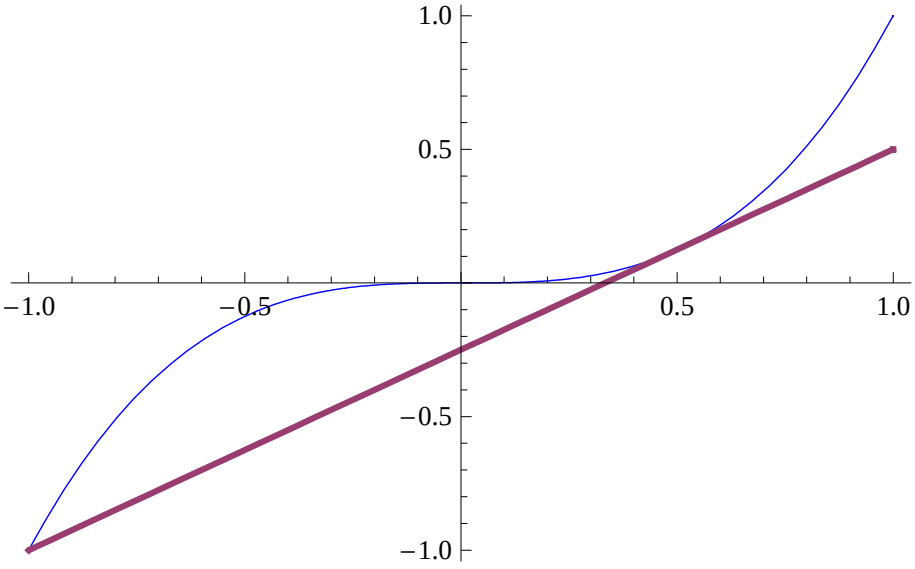


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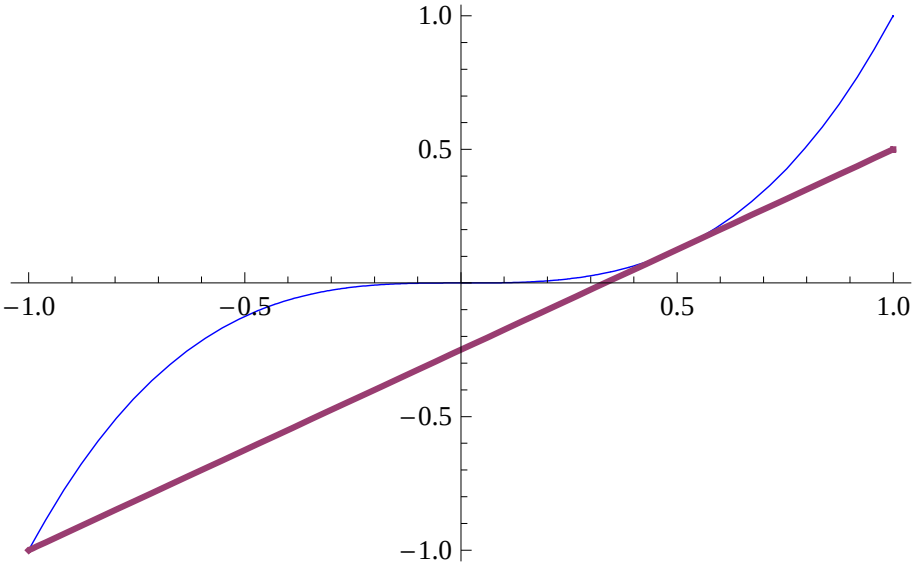


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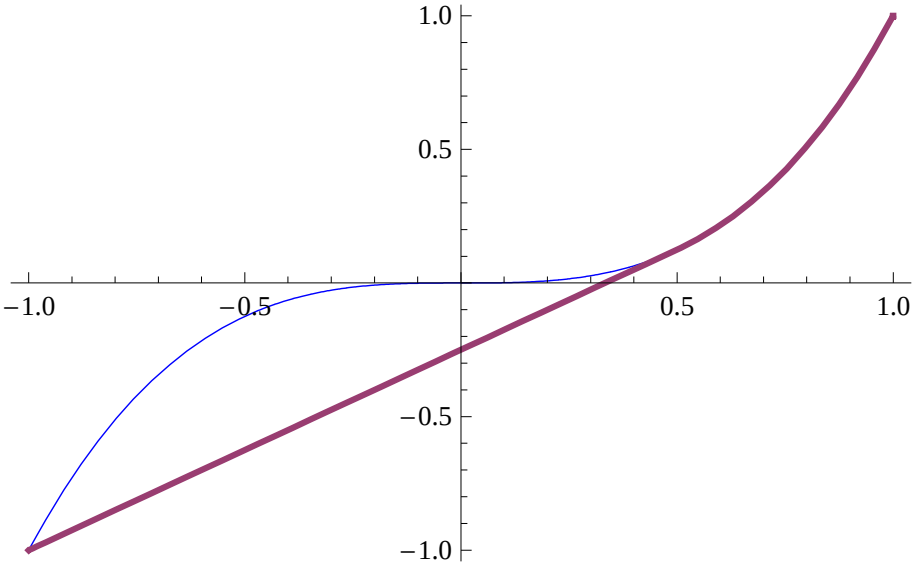


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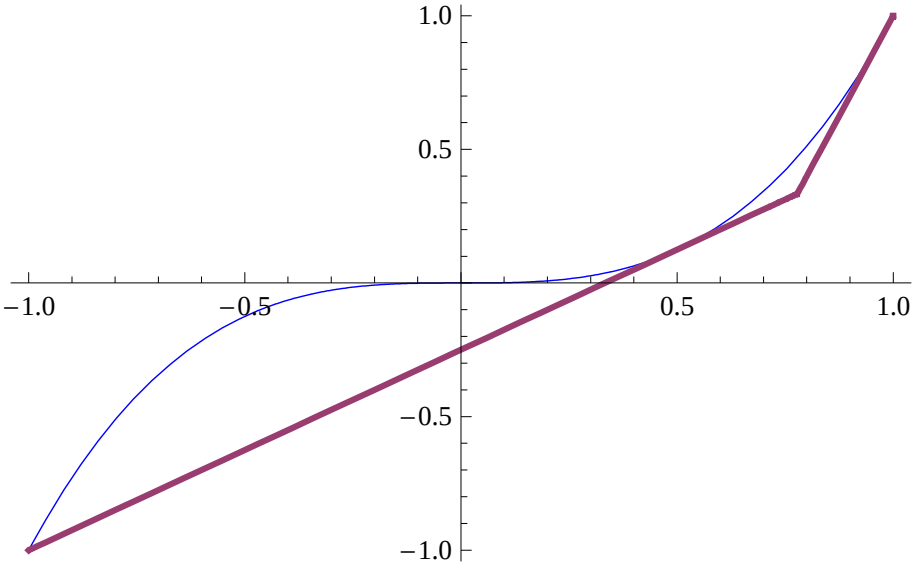


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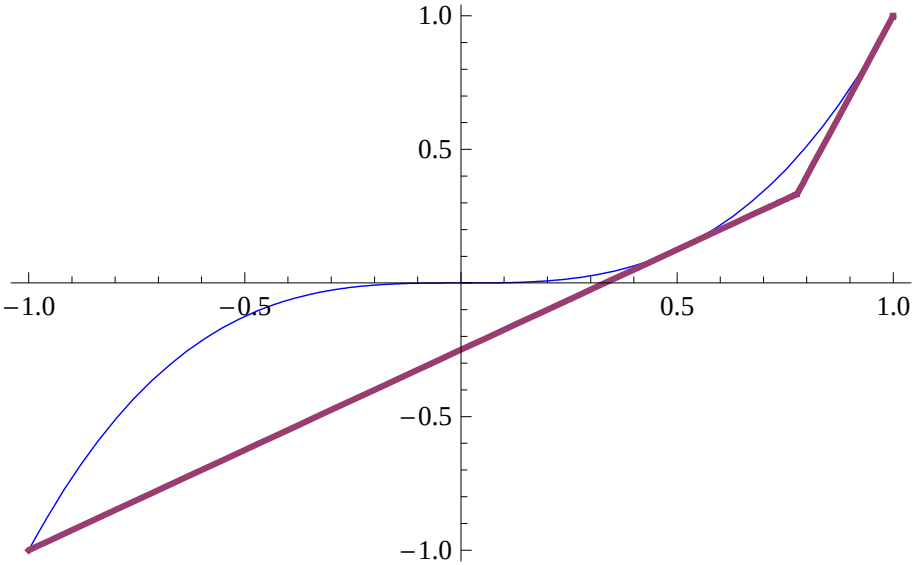


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- obtain convex envelope and linear approximation
- easily generalized to $x|x|^{n-1} = \text{sign}(x)|x|^n$, $n \geq 1$ (application for flow of water and gas in pipes)

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# Convex envelope for $x \cdot y$

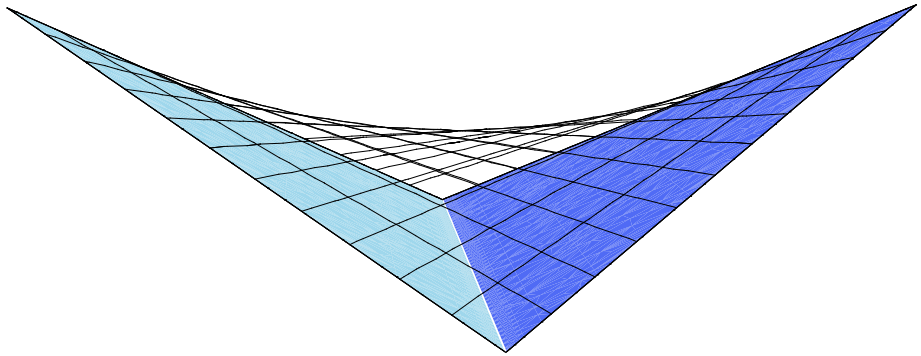
[McCormick, 1976]

McCormick: The convex envelope of

$$f(x) = xy$$

for $x \in [\underline{x}, \overline{x}]$, $y \in [\underline{y}, \overline{y}]$ is

$$xy \geq \max \left\{ \begin{array}{l} \overline{x}y + \overline{y}x - \overline{xy} \\ \underline{x}y + \underline{y}x - \underline{x}\underline{y} \end{array} \right\}$$



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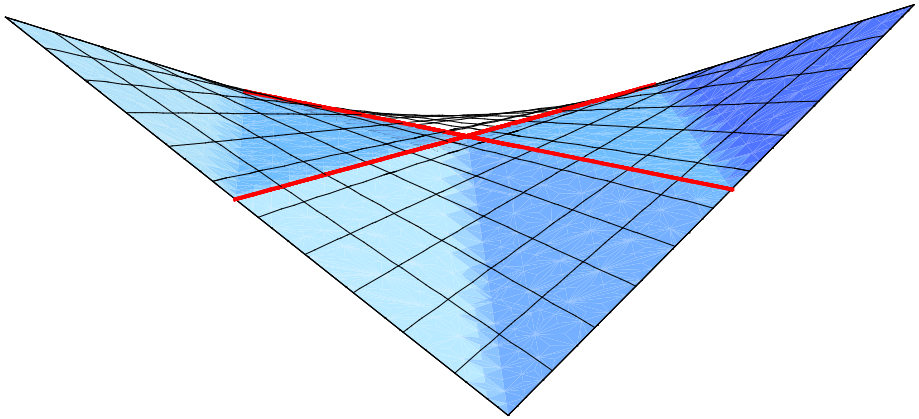

- apply McCormick underestimators to (nonconvex) quadratic forms

$$f(x) = \sum_{i,j} a_{i,j} x_i x_j$$

- branching on $x$ and $y$ changes variable bounds
  $\Rightarrow$ tighter underestimator $\Rightarrow$ improving dual bounds

# Reformulation for the general (factorable) case

[Tawarmalani and Sahinidis, 2004]

Let $g : \mathbb{R}^m \to \mathbb{R}$ be factorable, i.e., a recursive sum and product of univariate functions

Examples: $g(x) = x_1 x_2$, $g(x) = x_1/x_2$, $g(x) = \sqrt{\exp(x_1 x_2 + x_3 \ln x_4) x_3^3}$

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Reformulation: replace products of functions or variables by new variables

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\begin{aligned}
g &= \sqrt{\exp(y_1) y_2} \\
y_1 &= x_1 x_2 + x_3 \ln(x_4) \\
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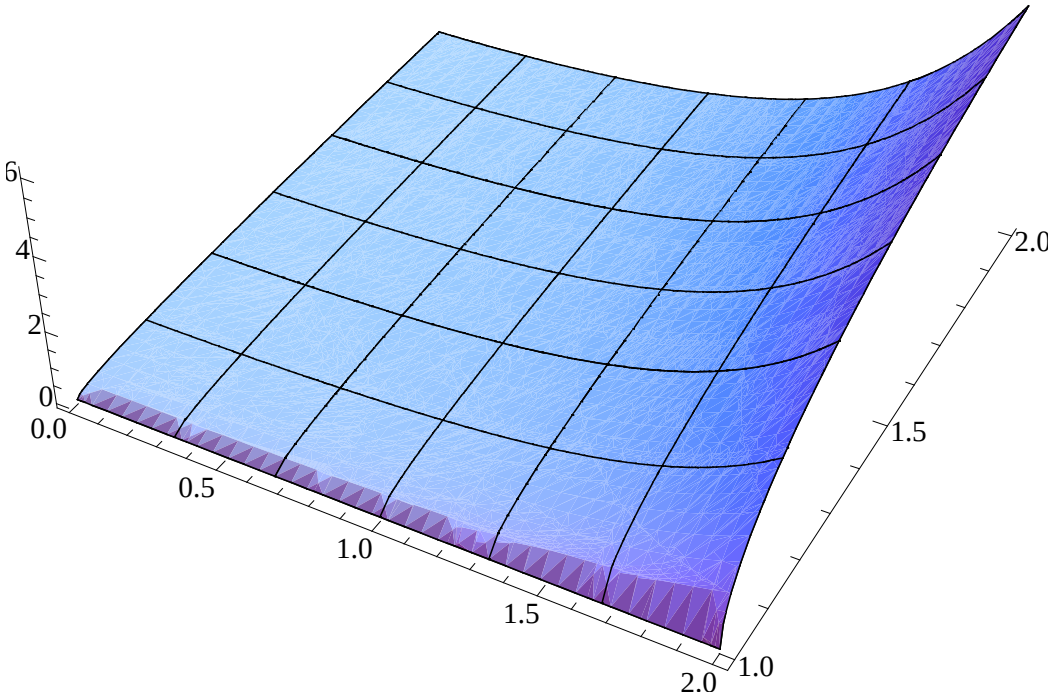
Convex outer-approximation by

- ▷ estimating univariate functions by known convex envelopes
- ▷ estimating bilinear terms by McCormick underestimators

# Example for convexification via factorable reformulation

$$g(x) = \sqrt{\exp(x_1^2)\ln(x_2)}$$

$$x_1 \in [0,2], \quad x_2 \in [1,2]$$



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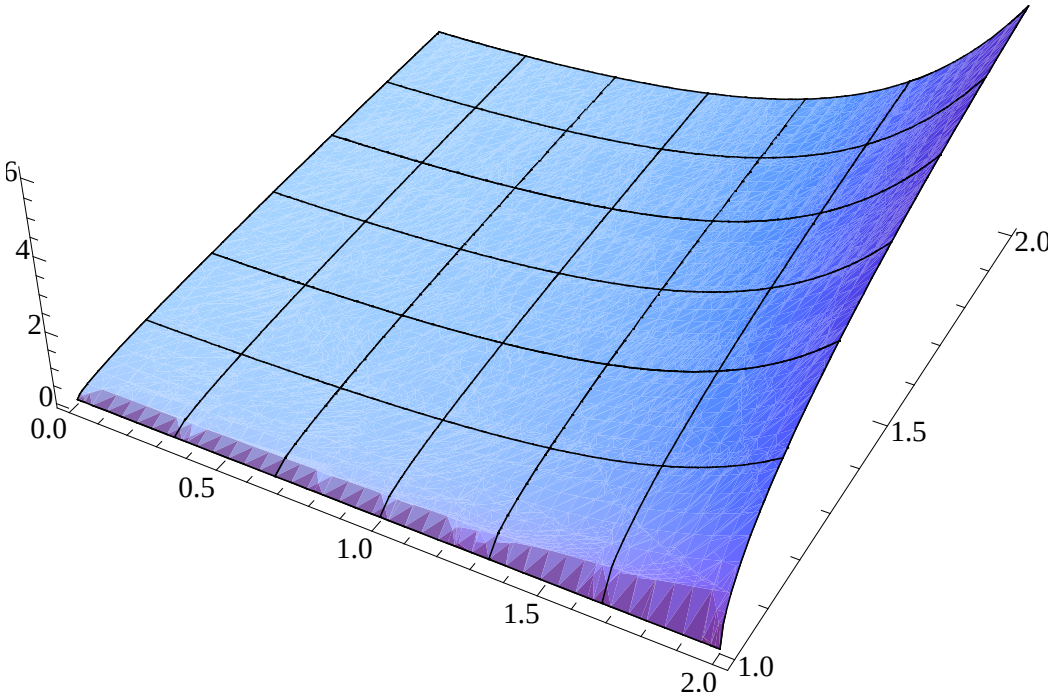

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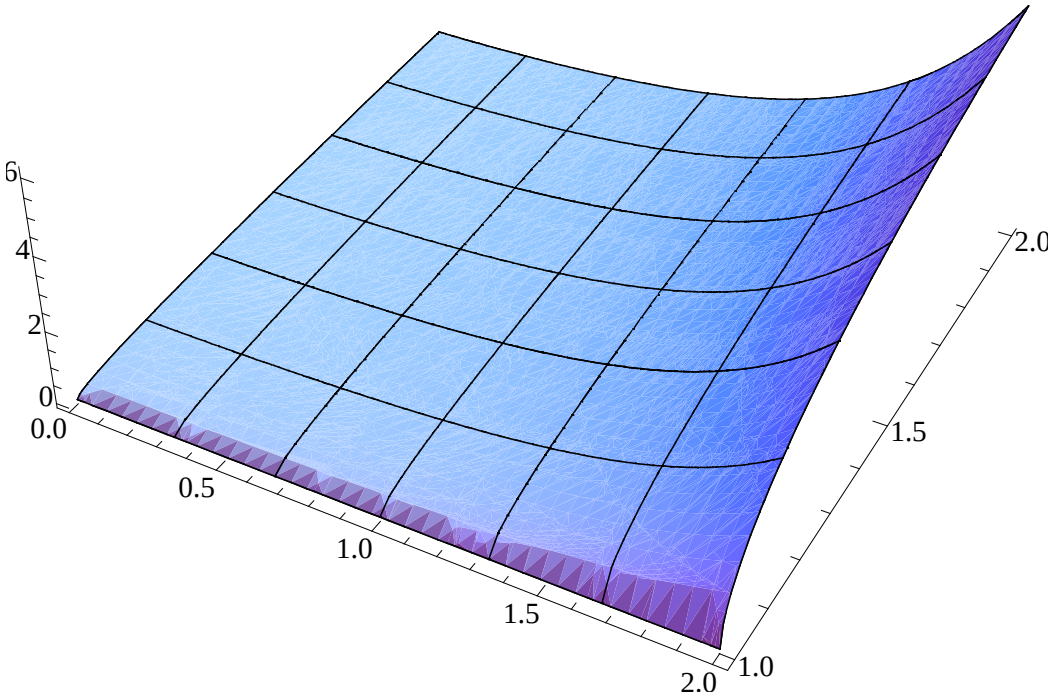

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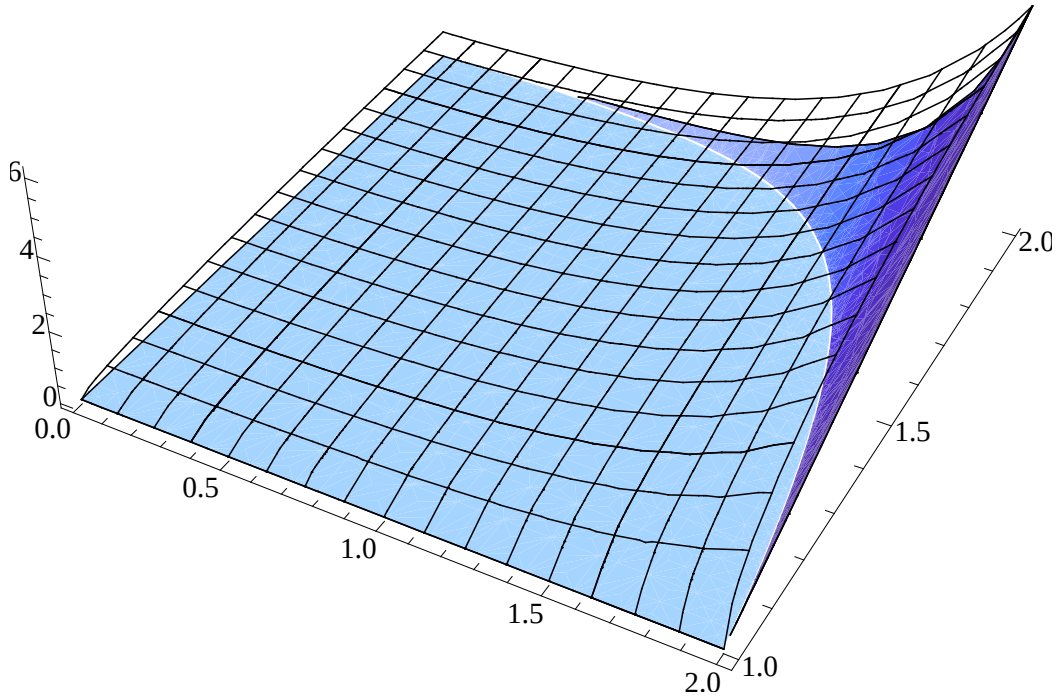


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Convex relaxation:

$$\sqrt{\underline{y_1}} + \frac{y_1 - \underline{y_1}}{\sqrt{\overline{y_1}} + \sqrt{\underline{y_1}}} \le g \le \sqrt{y_1}; \quad \ln \underline{x_1} + (x_2 - \underline{x_2})\frac{\ln \overline{x_2} - \ln \underline{x_2}}{\overline{x_2} - \underline{x_2}} \le y_3 \le \ln(x_2)$$

$$\max \left\{ \begin{array}{c} \overline{y_2} y_3 + \overline{y_3} y_2 - \overline{y_2 y_3} \\ \underline{y_2} y_3 + \underline{y_3} y_2 - \underline{y_2 y_3} \end{array} \right\} \le y_1 \le \min \left\{ \begin{array}{c} \overline{y_2} y_3 + \underline{y_3} y_2 - \overline{y_2}\,\underline{y_3} \\ \underline{y_2} y_3 + \overline{y_3} y_2 - \underline{y_2}\,\overline{y_3} \end{array} \right\}$$

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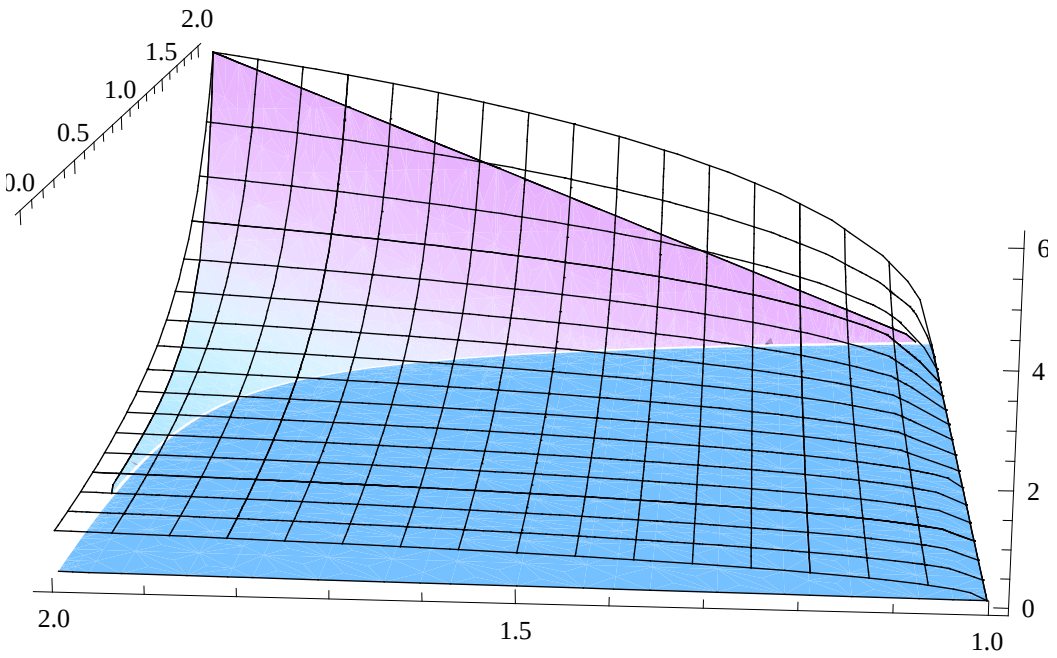


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$$\begin{aligned} g &= \sqrt{y_1} & \\ y_1 &= y_2 y_3 & [0, \ln(2)e^4] \\ y_2 &= \exp(y_4) & [1, e^4] \\ y_3 &= \ln(x_2) & [0, \ln(2)] \\ y_4 &= x_1^2 & [0, 4] \end{aligned}$$

Convex relaxation:

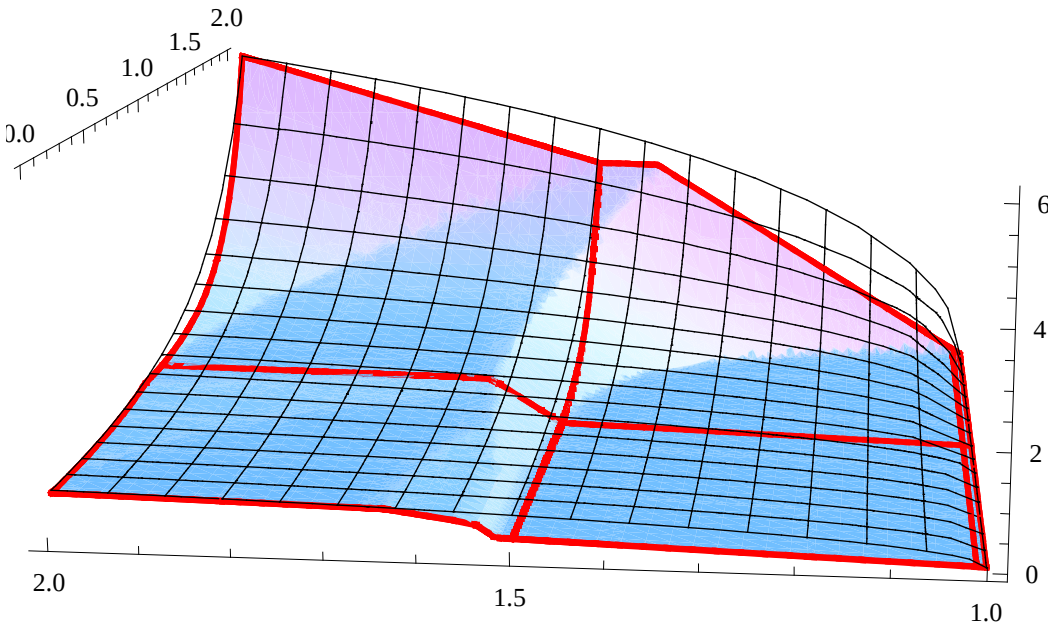
$$\sqrt{\underline{y_1}} + \frac{y_1 - \underline{y_1}}{\sqrt{\overline{y_1}} + \sqrt{\underline{y_1}}} \le g \le \sqrt{y_1}; \quad \ln \underline{x_1} + (x_2 - \underline{x_2})\frac{\ln \overline{x_2} - \ln \underline{x_2}}{\overline{x_2} - \underline{x_2}} \le y_3 \le \ln(x_2)$$

$$\max \left\{ \begin{array}{c} \overline{y_2} y_3 + \overline{y_3} y_2 - \overline{y_2 y_3} \\ \underline{y_2} y_3 + \underline{y_3} y_2 - \underline{y_2 y_3} \end{array} \right\} \le y_1 \le \min \left\{ \begin{array}{c} \overline{y_2} y_3 + \underline{y_3} y_2 - \overline{y_2}\,\underline{y_3} \\ \underline{y_2} y_3 + \overline{y_3} y_2 - \underline{y_2}\,\overline{y_3} \end{array} \right\}$$

...

# Example for convexification via factorable reformulation

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




Factorable Reformulation:

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# Outline

## BARON = Branch And Reduce Optimization Navigator

[Tawarmalani and Sahinidis, 2002]

- developed by N. Sahinidis, M. Tawarmalani
- state-of-the-art convexification techniques
- winner of Beale-Orchard-Hays Prize 2006

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## LindoGlobal

[Lin and Schrage, 2009]

- developed by Y. Lin and L. Schrage
- some automatic reformulation techniques (SOC, `floor`, `abs`, `max`, ...)

LINDO SYSTEMS INC.

# Solvers for nonconvex MINLP in Development

MINOTAUR = Mixed-Integer Nonconvex Optimization Toolbox – Algorithms, Underestimators, Relaxations [Mahajan and Munson, 2010]

- developed by A. Mahajan, T. Munson, et.al.
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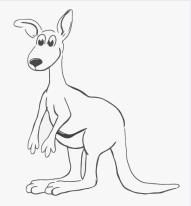
## SCIP = Solving Constraint Integer Programs [Berthold et al., 2009a]

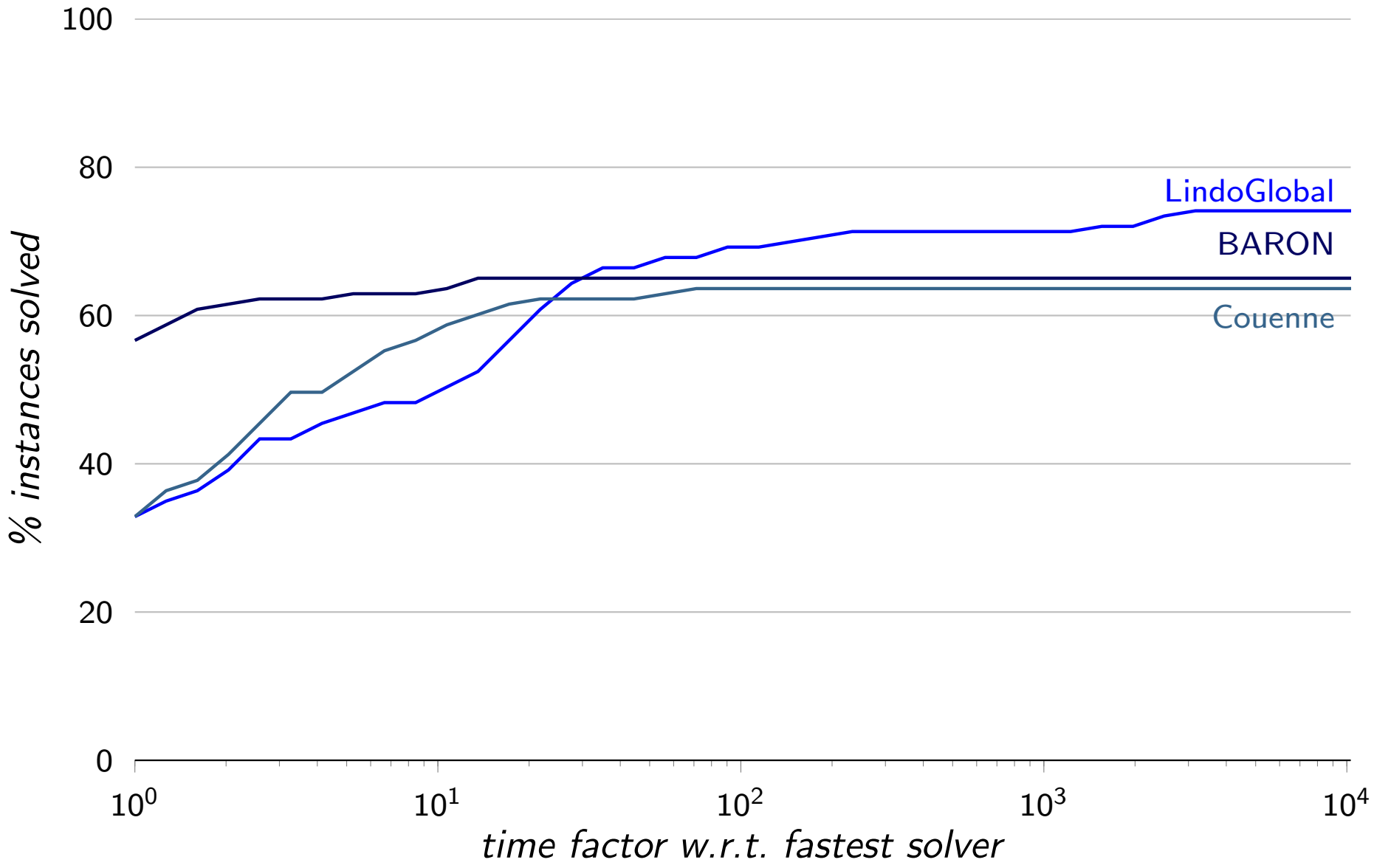
- support for MIQQP so far
- strong in MIP part



Experimental Environment:

- test set: 143 MINLP instances from MINLPLib [Bussieck et al., 2003]
  convex and nonconvex, easy and hard
- solvers:
  - BARON 9.0.8
    CPLEX for LPs and MINOS for NLPs
  - LindoGlobal 6.1.1
    CPLEX for LPs and CONOPT for NLPs
  - Couenne 0.3
    CLP for LPs and IPOPT for NLPs
- timelimit 1 hour, gap tolerance $10^{-4}$
- 3.0GHz Intel Core2 Extreme CPU X9650, 16GB RAM

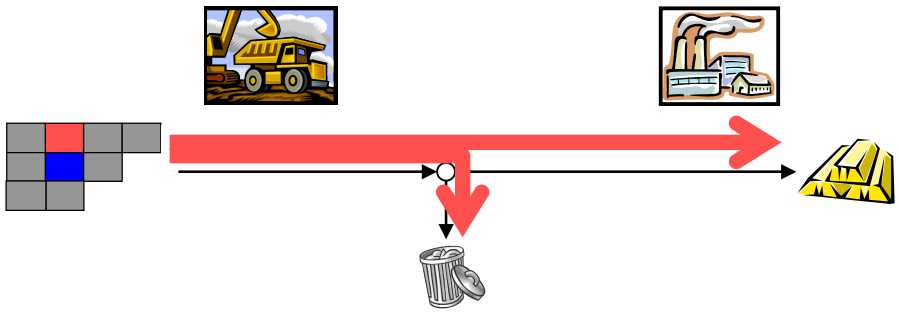
# Benchmark on 143 MINLPs



# Outline

## Open Pit Mine Production Scheduling with a Stockpile [Bley et al., 2009a]

# Open Pit Mine Production Scheduling – Basic Version



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

Given:

- Blocks (or aggregates)
  (rock, metal grade, precedences)
- Capacities, Costs
  (Mining, Processing; per rock ton)
- Metal Prices

Decisions:

- When to mine which block?
- Which block to process?

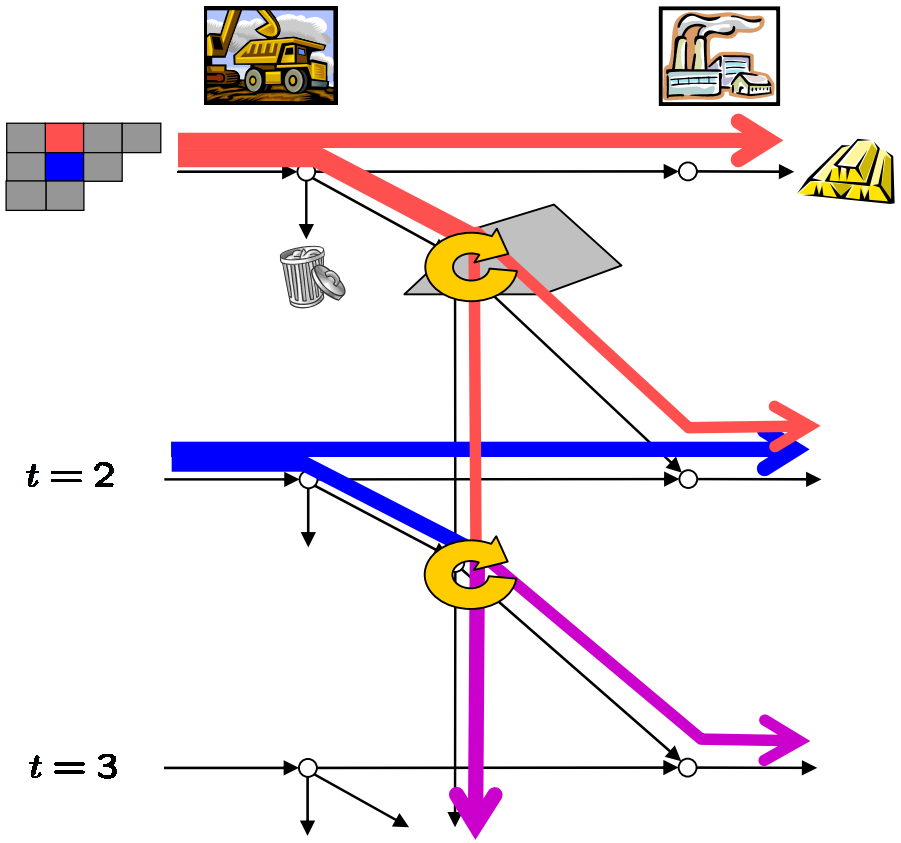
Goal:

max NPV

Solution Approach:

Time-indexed MILP formulation

# Open Pit Mine Production Scheduling with Stockpiles




Practical extension:

Stockpile for interim storage

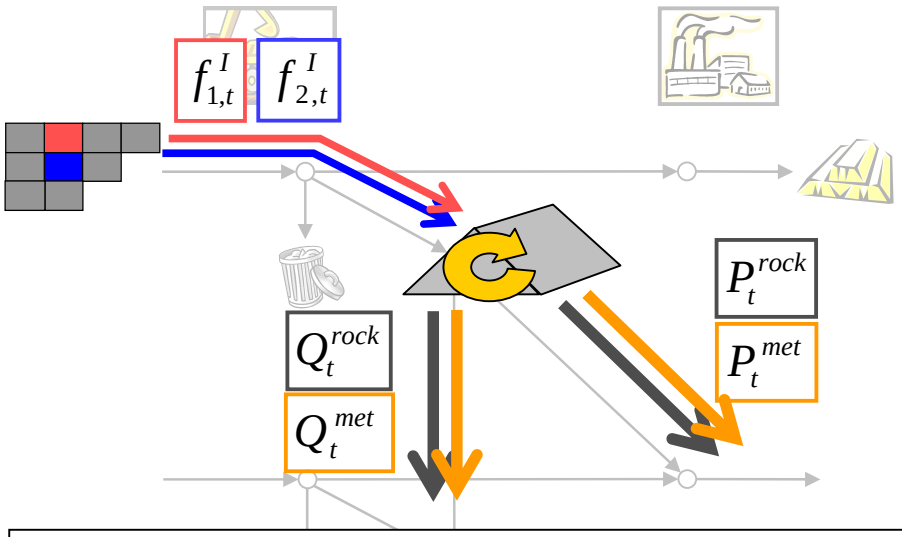
⇩

better use of capacities

Difficulty:

stockpile mixes material

# Open Pit Mine Production Scheduling with Stockpiles




Aggregated stockpile model

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

$Q^{rock}_t, Q^{met}_t$ total rock / metal tons held

$P^{rock}_t, P^{met}_t$ total rock / metal tons out

Mixing constraints:

$$\frac{P^{met}_t}{Q^{met}_t} = \frac{P^{rock}_t}{Q^{rock}_t}$$

(metal fraction out = rock fraction out)

## Practical extension:

Stockpile for interim storage

⇩

better use of capacities

## Difficulty:

stockpile mixes material

## Mathematical model:

Same rock / metal – mix held and taken out of stockpile

⇩

Nonlinear constraints

# Aggregate MINLP formulation

$$\max \quad \sum_{t \in years} \left[ v_t \left( P_t^{met} + \sum_{i \in blocks} \alpha_i^{met} f_{i,t}^P \right) - c_t^P \left( P_t^{rock} + \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^P \right) - c_t^M \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^M \right]$$

s.t.

$$\left.\begin{aligned} \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^M &\le MC_t \qquad \forall\, t \\ P_t^{rock} + \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^P &\le PC_t \qquad \forall\, t \end{aligned}\right\} \text{Capacities}$$

$$\left.\begin{aligned} \sum_{s=1,\ldots,t} f_{i,s}^M &\ge x_{i,t} \qquad \forall\, t,\ i \\ \sum_{s=1,\ldots,t} f_{i,s}^M &\le x_{j,t} \qquad \forall\, t,\ j \in \mathrm{Pred}(i) \end{aligned}\right\} \text{Precedences}$$

$$\left.\begin{aligned} \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^I + Q_t^{rock} - Q_{t+1}^{rock} - R_{t+1}^{rock} &= 0 \qquad \forall\, t \\ &\vdots \end{aligned}\right\} \text{Flow balance}$$

$$P_t^{met} Q_t^{rock} - Q_t^{met} P_t^{rock} = 0 \qquad \forall\, t \qquad \text{— Stockpile mixing}$$

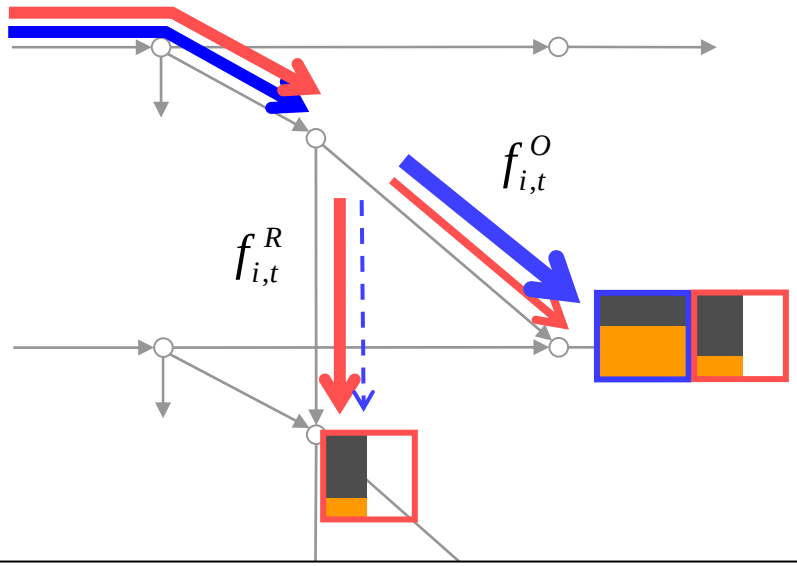
$$0 \le f_{i,t}^* \le 1$$

$$P_t^*, Q_t^* \ge 0$$

$$x_{i,t} \in \{0,1\}$$

# Extended MINLP formulation

- track each block's fractions individually through the stockpile
- best possible knowledge of the material in the stockpile




$f_{i,t}^{O} \in [0,1]$ % of block i out of stockpile

$f_{i,t}^{R} \in [0,1]$ % of block i kept in stockpile

$$P_t^{rock} = \sum_{i \in blocks} \alpha_i^{rock} f_{i,t}^{O}$$ total rock out

$\vdots$

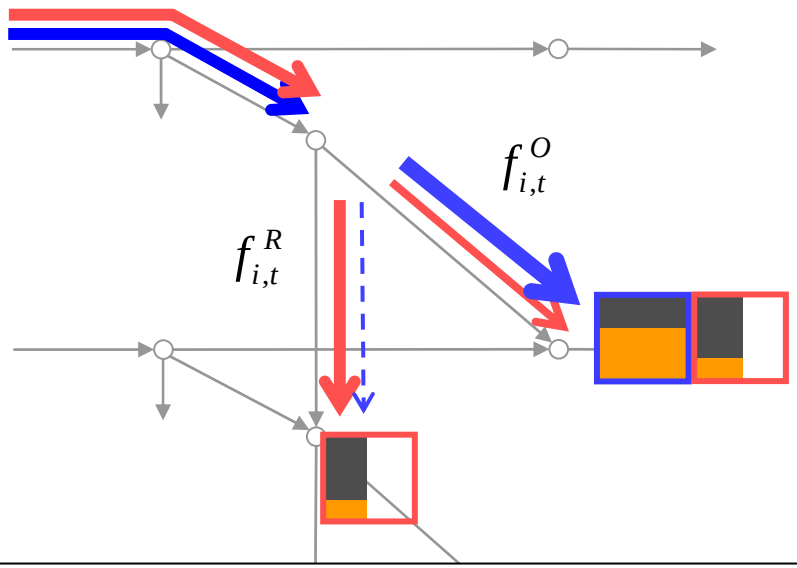
# Extended MINLP formulation

- track each block's fractions individually through the stockpile
- best possible knowledge of the material in the stockpile
- require

$$\frac{f_{i,t}^{O}}{f_{i,t}^{O} + f_{i,t}^{R}} = r_t$$

for each period and block

$\Rightarrow$ much tighter dual bound

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- ignore nonlinearities to obtain linear relaxation
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How close can generic MINLP solvers get without problem-specific knowledge? [Bley et al., 2009b]

# SCIP: Handling bilinear constraints

- Mixing constraints:

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- McCormick underestimators provide a linear outer approximation for each bilinear term $(xy)$:

$$\begin{aligned}
xy &\geq \underline{x}y + \underline{y}x - \underline{x}\underline{y} \\
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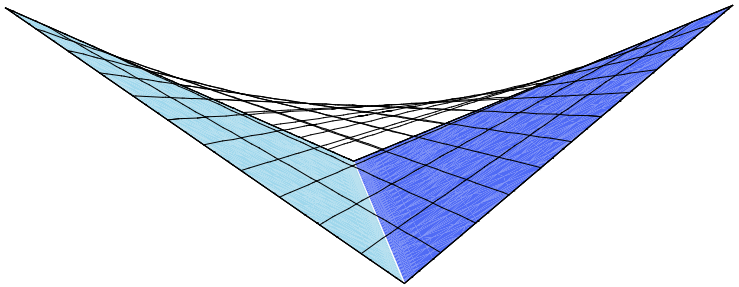

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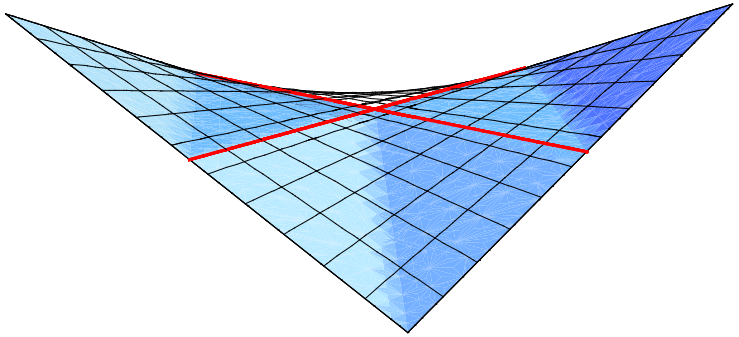

- Separate dynamically if violated, otherwise perform spatial branching

# SCIP: Producing feasible solutions

Primal solutions from: feasible LP solution, MIP heuristics, NLP local search, extended LNS heuristics

New heuristic: Undercover [Berthold and Gleixner, 2009]

- idea: fix variables such as to obtain a linear subproblem
- generic: solve an auxiliary set covering problem to automatically detect a minimal set of variables to fix
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Here: Fixing only $r_1, \ldots, r_T$ linearises the mixing constraints

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Expensive, but effective heuristic: produces fully feasible solutions within 1% of the global optimum.

# Problem-specific vs. generic algorithms

Compare the performance of

- BARON 9.0.2
- Couenne 0.2
- SCIP 2.0

to the CPLEX-based implementation of Bley et al. [2009a],

Compare the performance of

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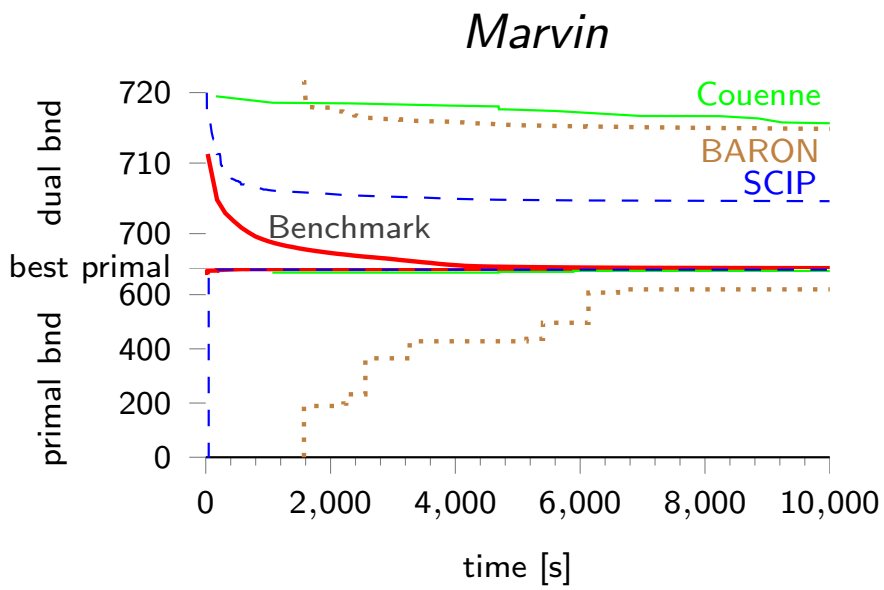
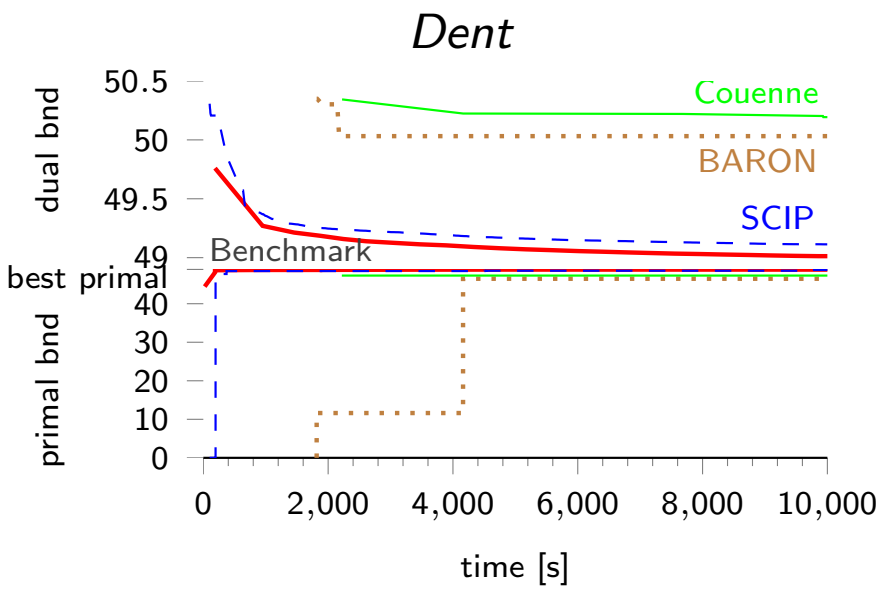
to the CPLEX-based implementation of Bley et al. [2009a],
on 2 realistic mine production scheduling instances from industry:

| | *Marvin* | | | | *Dent* | | | |
|---|---|---|---|---|---|---|---|---|
| | no. variables | | no. constraints | | no. variables | | no. constraints | |
| | bin | cont | linear | quad | bin | cont | linear | quad |
| aggreg. model | 1445 | 4403 | 7582 | 16 | 3125 | 9475 | 15750 | 24 |
| ext. model | 1445 | 7242 | 9044 | 1360 | 3125 | 15650 | 18900 | 3000 |




- benchmark algo. closes gap up to 0.02% (Marvin) and 0.33% (Dent) after 10000 secs
- SCIP (with LP solver CPLEX) reaches 1.80% resp. 0.71%
- difference is also due to
  - underlying MIP solver (CPLEX vs. SCIP)
  - problem-specific MIP cuts/variable fixings

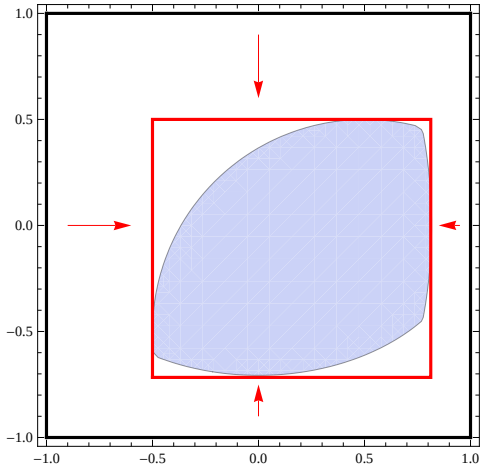
  i.e. not only/mainly due to the handling of the nonlinearities.

# Outline

# Bounds Tightening (Domain Propagation)

Tighten variable bounds $[\underline{x}, \overline{x}]$ such that

- the optimal value of the problem is not changed, or
- the set of optimal solutions is not changed, or
- the set of feasible solutions is not changed



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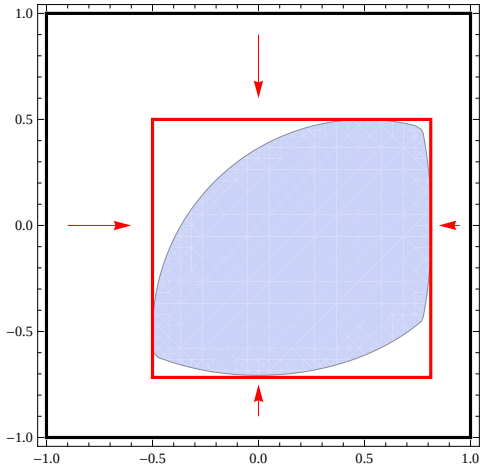


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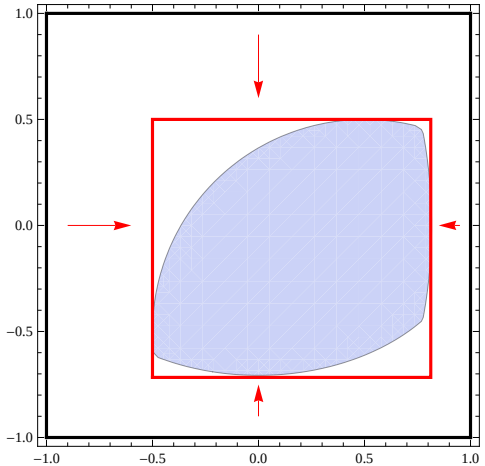


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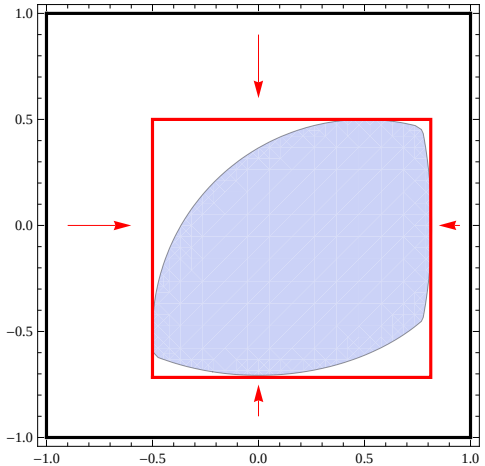


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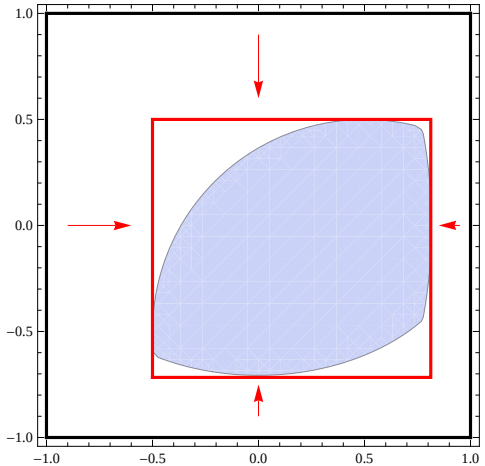


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Some techniques [Belotti et al., 2009]:

FBBT Feasibility-Based Bounds Tightening (cheap)

ABT Aggressive Feasibility-Based Bounds Tightening (expensive)

OBBT Optimality-Based Bounds Tightening (expensive)

# FBBT for Linear Constraints

Feasibility-Based Bound Tightening for a linear constraint:

$$\underline{b} \leq \sum_{i:a_i>0} a_i x_i + \sum_{i:a_i<0} a_i x_i \leq \overline{b},$$

Feasibility-Based Bound Tightening for a linear constraint:

$$\underline{b} \leq \sum_{i:a_i>0} a_i x_i + \sum_{i:a_i<0} a_i x_i \leq \overline{b},$$

$$\Rightarrow \quad x_j \leq \frac{1}{a_j} \begin{cases} \overline{b} - \sum_{i:a_i>0, i\neq j} a_i \underline{x}_i - \sum_{i:a_i<0} a_i \overline{x}_i, & \text{if } a_j > 0 \\ \underline{b} - \sum_{i:a_i>0} a_i \overline{x}_i - \sum_{i:a_i<0, i\neq j} a_i \underline{x}_i, & \text{if } a_j < 0 \end{cases}$$

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$$\sqrt{x} + 2\sqrt{xy} + 2\sqrt{y} \in [-\infty, 7]$$
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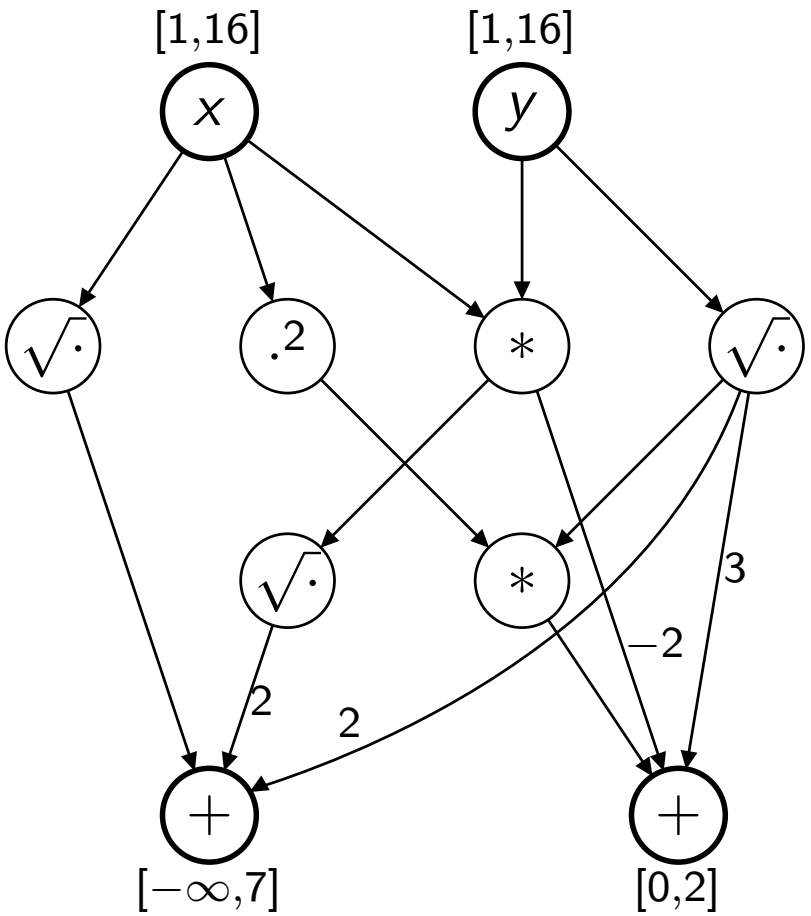
$$x, y \in [1, 16]$$



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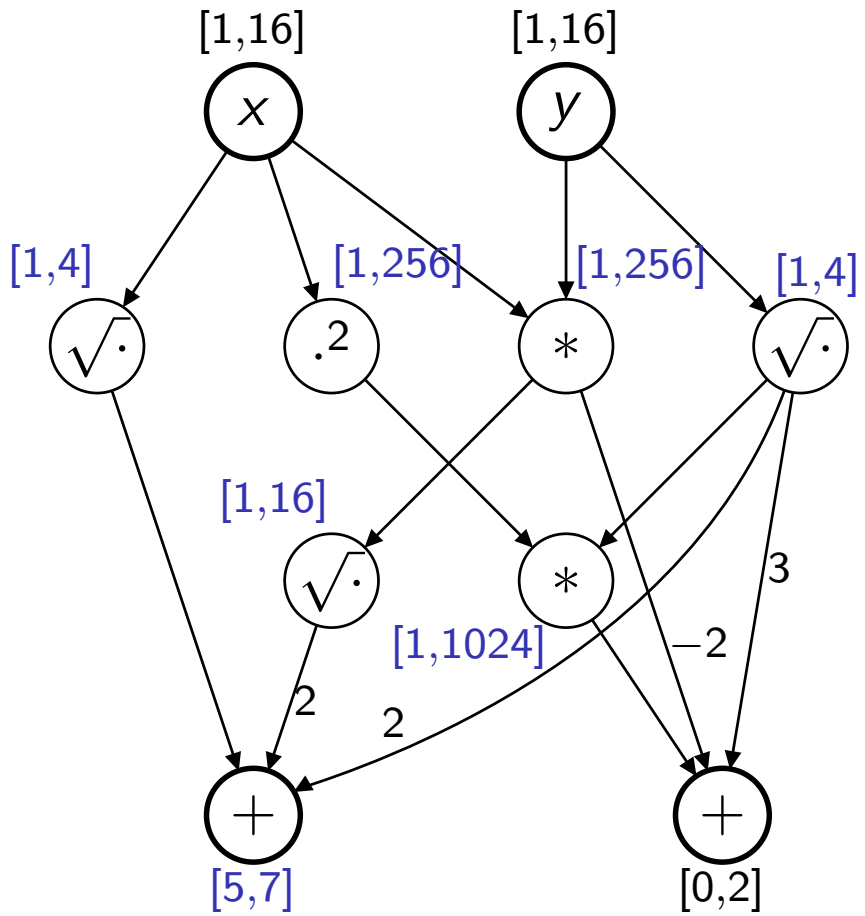

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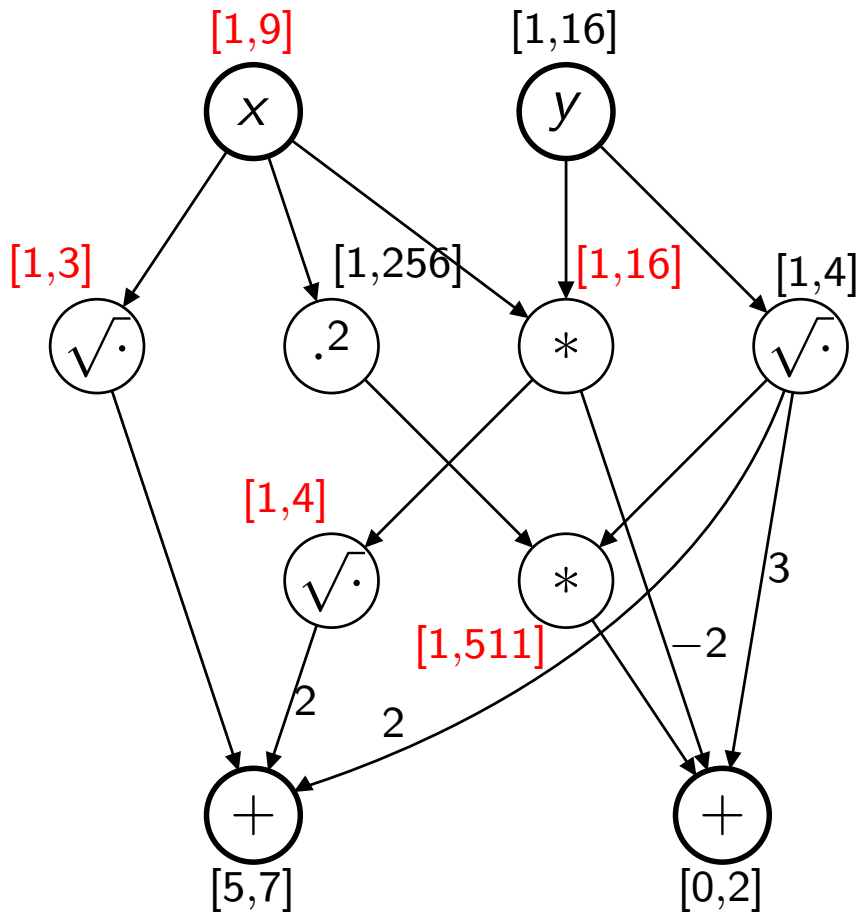


Forward propagation:

- compute bounds on intermediate nodes (top-down)

Backward propagation:

- reduce bounds using reverse operations (bottom-up)

## Probing for MIP

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- tentatively reduce bounds of a nonlinear variable, e.g., $x_i \leq 0.3\overline{x}_i$, and apply FBBT
- if infeasibility is detected, tighten bound in main problem, e.g., $\underline{x}_i := 0.3\overline{x}_i$

# Aggressive Bound Tightening

## Probing for MIP

- tentatively fix binary variable $x_i$ and apply domain propagation
- if infeasibility is detected for $x_i = a$, then fix binary variable to $1 - a$ in main problem
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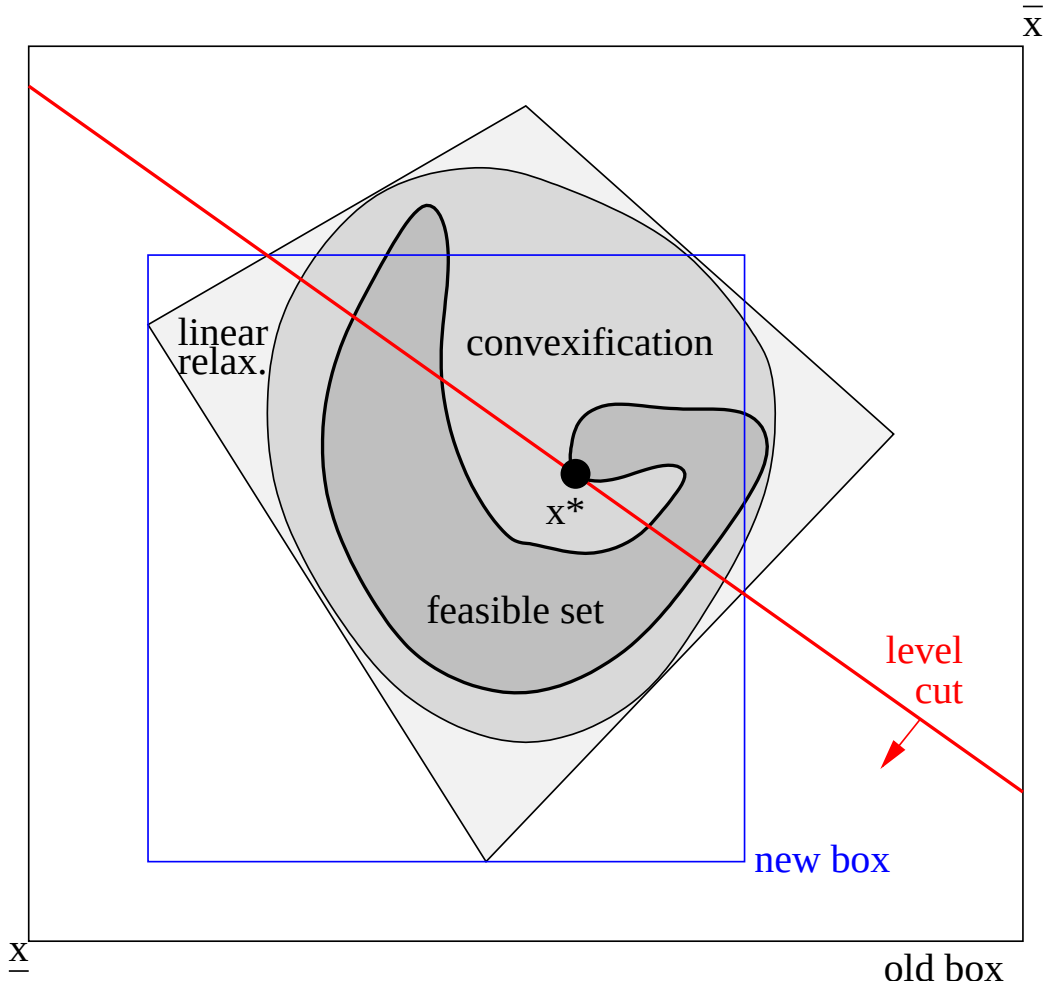
- tentatively reduce bounds of a nonlinear variable, e.g., $x_i \leq 0.3\overline{x}_i$, and apply FBBT
- if infeasibility is detected, tighten bound in main problem, e.g., $\underline{x}_i := 0.3\overline{x}_i$
- within B&B: update and solve LP relaxation to obtain lower bound for tentative reduction

# Optimality-Based Bound Tightening

- Consider a linear relaxation with constraints $Ax \leq b$.
- Let $x^*$ be the best solution found so far.

$$\underline{x}_i := \min x_i \quad \text{s.t. } Ax \leq b, \quad c^T x \leq c^T x^*$$

$$\overline{x}_i := \max x_i \quad \text{s.t. } Ax \leq b, \quad c^T x \leq c^T x^*$$



# Bound Tightening Methods: Computational Study

## Effect of disabling FBBT in SCIP on 89 MIQQPs [Berthold et al., 2010]

- number of instances solved: $-1$
- mean running time: $+6\%$
- time to first / optimal solution: $+13\%$ / $+7\%$
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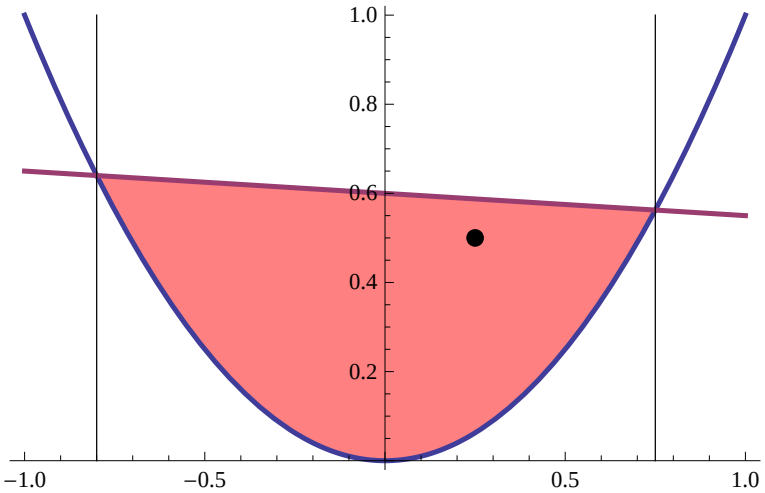
## Effect of bound tight. in Couenne on 21 (MI)NLPs [Belotti et al., 2009]

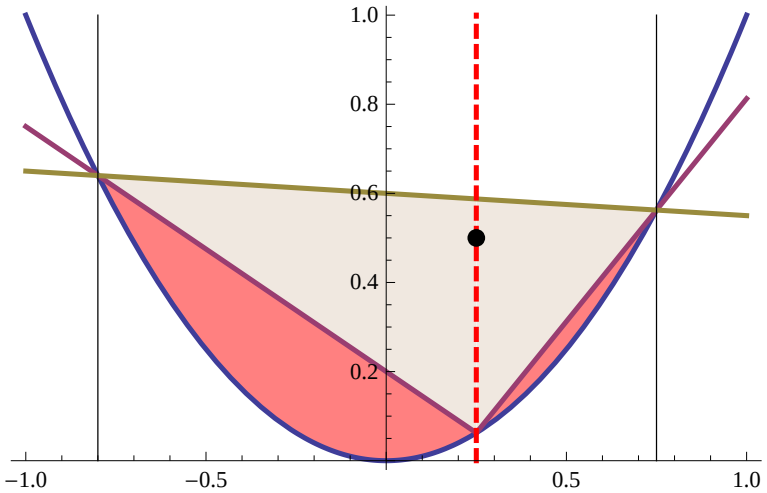
| Method | #solved | #best time | #best nodes | #best depth |
|---|---|---|---|---|
| FBBT + ABT + OBBT* | 19 | 12 | 14 | 16 |
| FBBT only | 16 | 2 | 4 | 6 |
| FBBT + ABT** | 14 | 1 | 3 | 6 |
| no bound tightening | 16 | 10 | 7 | 10 |
| FBBT + OBBT*** | 16 | 2 | 8 | 9 |

* "tuned" = apply ABT and OBBT at root or with prob. $2^{1-\text{depth}}$ and $2^{-\text{depth}}$, resp.
** apply ABT at root or with prob. $2^{3-\text{depth}}$, if depth $> 3$
*** apply OBBT at root or with prob. $2^{3-\text{depth}}$, if depth $> 3$

Branching in MINLP:

- on an integer variable to resolve fractionality
- on a nonlinear variable in a nonconvex term to allow tighter relaxation



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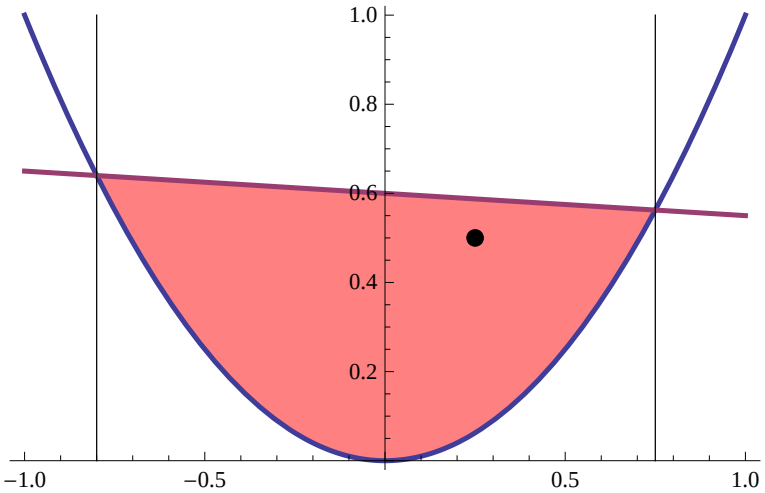


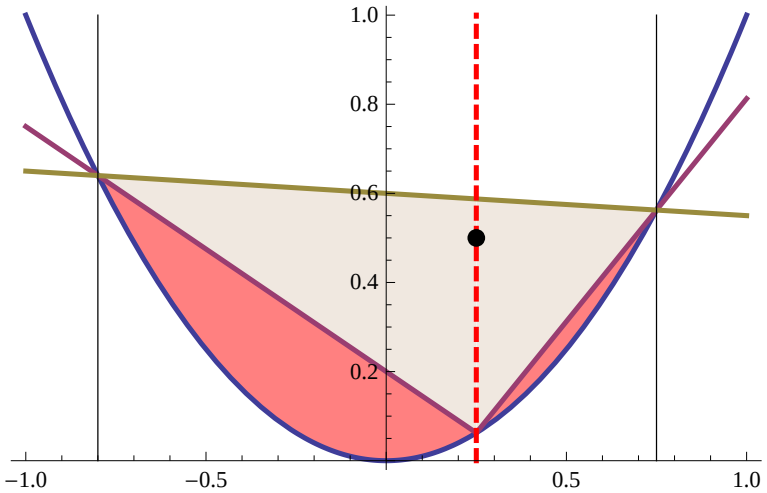


**How to select the branching variable from a set of variable candidates?**

- give priority to integer variables
  apply MIP branching techniques (most fractional, reliability branching, strong branching, ...)
- extend these branching rules to continuous variables [Belotti et al., 2009]

# Branching Rule: Most violated

## "Most fractional" rule for integer variables

Branch on $x_{i^*}$, such that

$$i^* = \text{argmax}_{i \in I} \ \min\{\hat{x}_i - \lfloor \hat{x}_i \rfloor, \lceil \hat{x}_i \rceil - \hat{x}_i\},$$

where $\hat{x}$ is the current solution of the LP relaxation.

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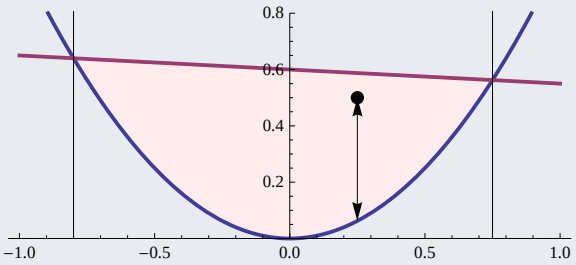
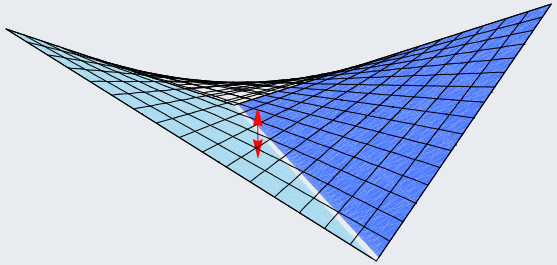
## "Most violated" rule for nonlinear variables [Belotti et al., 2009]

Assign to each variable $x_i$ the set of "convexification gaps" $U_{i,j}(\hat{x})$ in $\hat{x}$ for all nonconvex terms $j$ in which $x_i$ is involved



Branch on $x_{i^*}$, such that

$$i^* = \text{argmax}_{i \in I} \ \frac{1}{10} \sum_j U_{i,j}(\hat{x}) + \frac{13}{10} \max_j U_{i,j}(\hat{x}) + \frac{8}{10} \min_j U_{i,j}(\hat{x})$$

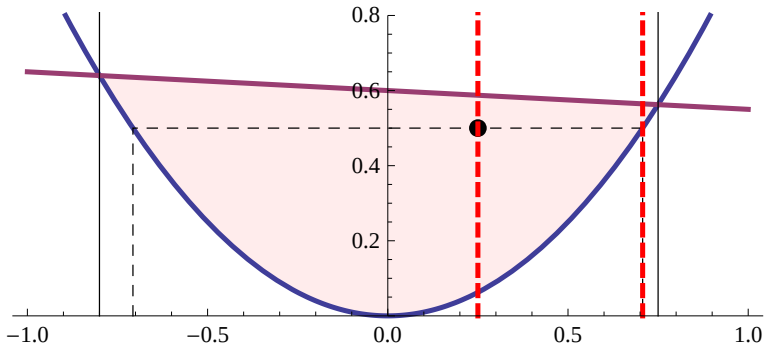
# Branching Rule: Violation transfer

[Tawarmalani and Sahinidis, 2004, Belotti et al., 2009]

Given $(\hat{x}, \hat{\pi})$ primal-dual solution of LP relaxation $Ax \leq b$, $A = (a_{ji})_{i,j}$.

For $x_i$, let $[\underline{\underline{x}}_i, \overline{\overline{x}}_i] \subseteq [\underline{x}_i, \overline{x}_i]$, s.t.

- $\hat{x}_j \in [\underline{x}_i, \overline{x}_i]$, and
- for every $x_j$, $x_j = f(x_i)$ (for some $f$), $\exists v \in [\underline{\underline{x}}_i, \overline{\overline{x}}_i] : f(v) = \hat{x}_j$, and
- as small as possible

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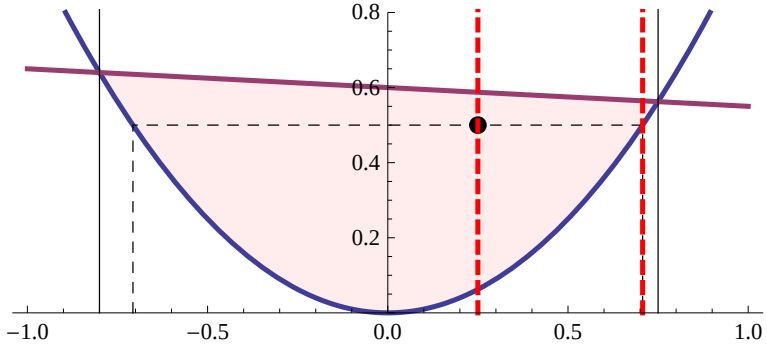


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Consider segment $\quad X_i := \{x : x_j = \hat{x}_j, j \neq i,\ x_i \in [\underline{\underline{x}}_i, \overline{\overline{x}}_i]\}$.

Estimate change in lower bound by range of Lagrange function of LP relaxation w.r.t. $X_i$:

$$\max_{x \in X_R^i} \mathcal{L}(x) - \min_{x \in X_R^i} \mathcal{L}(x) = |\overline{\overline{x}}_i - \underline{\underline{x}}_i| \, |\textstyle\sum_j \hat{\pi}_j a_{ji}|.$$

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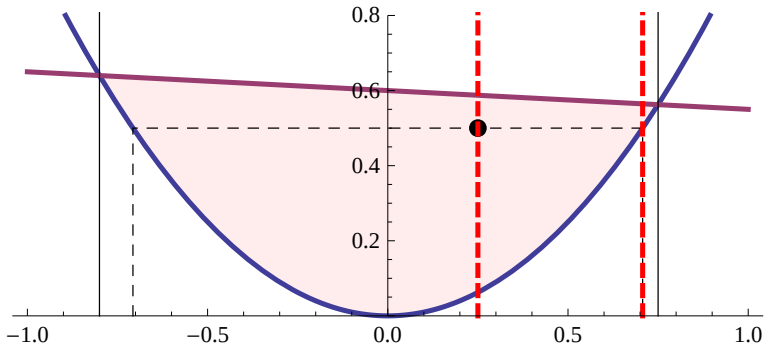


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**Integer variables $x_i$, $i \in I$**

- ▷ when branching, memorize resulting change in lower bound
- ▷ average bound improvements over all down- and up-branches of $x_i$ so far

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- Belotti et al. [2009] proposed several alternatives:
  - multiply pseudocosts by variable infeasibility (analog to fractionality):
    $$\psi_i^{-,+}\left(\tfrac{1}{10}\textstyle\sum_j U_{i,j}(\hat{x}) + \tfrac{13}{10}\max_j U_{i,j}(\hat{x}) + \tfrac{8}{10}\min_j U_{i,j}(\hat{x})\right)$$
  - multiply by domain width after branching:
    $$\psi_i^-(\hat{x}_i - \underline{x}_i),\ \psi_i^+(\overline{x}_i - \hat{x}_i) \quad \text{or} \quad \psi_i^-(\overline{x}_i - \hat{x}_i),\ \psi_i^+(\hat{x}_i - \underline{x}_i)$$
  - multiply by width of intervals from violation transfer:
    $$\psi_i^-(\hat{x}_i - \underline{\underline{x}}_i),\ \psi_i^+(\overline{\overline{x}}_i - \hat{x}_i)$$

# Branching Rule: Reliability Branching

## Strong Branching

- at each node, compute lower bound for all (or many) possible branchings (i.e., construct two branches, update and solve relaxation) and choose the one with best bound improvement
- expensive, but best reduction in number of nodes

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## Reliability branching

- compute exact bound improvement only for variables with a low number of branchings so far
- otherwise, assume pseudo costs are reliable and use them to evaluate potential bound improvement

$\Rightarrow$ initialization of pseudo costs by strong branching

Effect of branching techniques in Couenne on 33 (MI)NLPs [Belotti et al., 2009]:

| Method | #solved | #best time | #best nodes | #largest depth |
|---|---|---|---|---|
| variable infeasibility | 23 | 14 | 7 | 15 |
| violation transfer | 26 | 13 | 4 | 20 |
| rel.br.-var.infeas.* | 23 | 11 | 4 | 8 |
| rel.br.-dom.width** | 25 | 9 | 5 | 8 |
| strong branching | 25 | 1 | 17 | 11 |

* "rel.br.-infeas." = reliability branching with variable infeasibilities as pseudo costs multipliers

** "rel.br.-width" = reliability branching with domain width after branching as pseudo costs multipliers: $\psi_i^-(\overline{x}_i - \hat{x}_i)$, $\psi_i^+(\hat{x}_i - \underline{x}_i)$

# Reformulations for MIQCPs: SOC

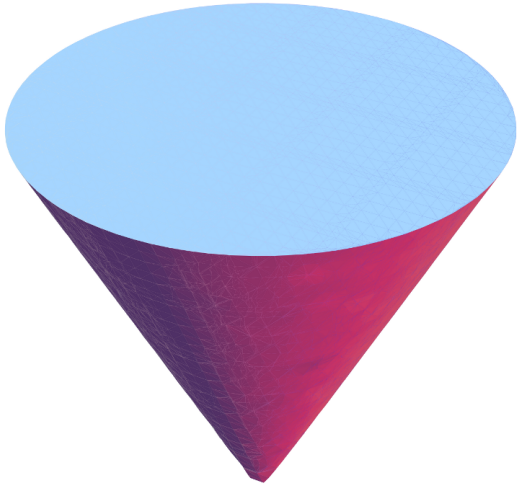
Quadratic constraints of the form

$$\sum_{k=1}^{N} \alpha_k x_k^2 - \alpha_{N+1} x_{N+1}^2 \leq 0$$

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

$$\sqrt{\sum_{k=1}^{N} \alpha_k x_k^2} \leq \sqrt{\alpha_{N+1}} x_{N+1}$$

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



feasible region

"ice cream cone"

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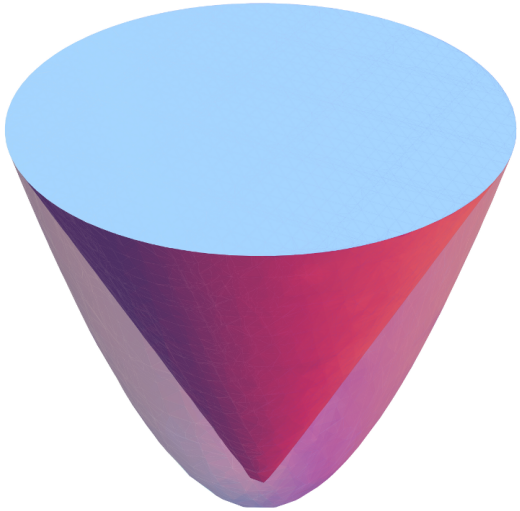

not recognizing SOC:
using termwise underestimator:

$$\left\{ \begin{array}{c} x^2 + y^2 + w \leq 1 \\ \frac{\underline{z}^2 - \overline{z}^2}{\overline{z} - \underline{z}}(z - \underline{z}) - \underline{z}^2 \leq w \end{array} \right\}$$

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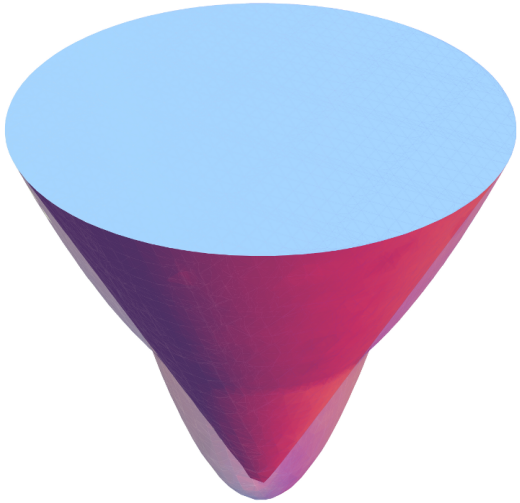
$$\sqrt{\sum_{k=1}^{N} \alpha_k x_k^2} \leq \sqrt{\alpha_{N+1}} x_{N+1}$$

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



not recognizing SOC:
using termwise underestimator:

$$\left\{ \begin{array}{c} x^2 + y^2 + w \leq 1 \\ \frac{\underline{z}^2 - \overline{z}^2}{\overline{z} - \underline{z}}(z - \underline{z}) - \underline{z}^2 \leq w \end{array} \right\}$$

after branching on $z = 0.5$

# Reformulations for MIQCPs: SOC

Quadratic constraints of the form

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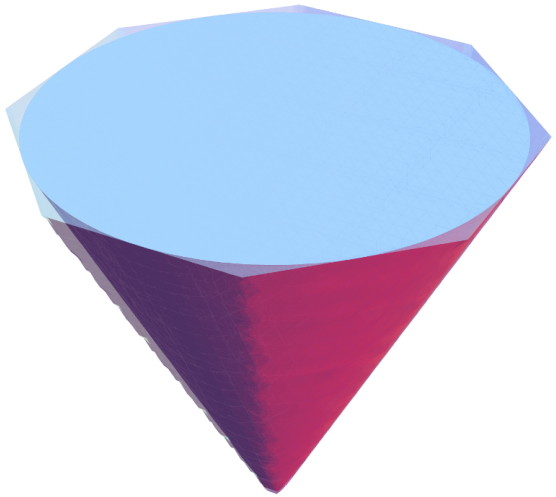

recognizing SOC:

initial relaxation
no spatial branching necessary

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- If $|\{i : E_{ii} < 0\}| = 0$, then quadratic function is convex.
- If $|\{i : E_{ii} < 0\}| = 1$ (w.l.o.g. $E_{11} < 0$) and $h := d - \frac{1}{4}\sum_i \text{sign}(D_{ii}) b_i^2 \geq 0$, then constraint is equivalent to

$$\left\| \begin{pmatrix} E_+(y + \frac{b}{2}) \\ \sqrt{h} \end{pmatrix} \right\|_2 \leq \left| y_1 - \frac{b_1}{2} \right|,$$

  where $E$ is diagonal matrix with $E_{ii}^+ = \max(0, E_{ii})$.
- Thus, constraint is equivalent to a union of two second order cones.

# Reformulations for MIQCPs: Convexify 0-1 QCPs

Assume $x \in \{0,1\}^n$ and consider the quadratic function

$$x^T A x, \quad \text{with} \quad A \not\succeq 0.$$

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|---|---|---|---|
| qap | -1171771 | 79071 | 388214 |
| pb302035 | -13223300 | 1151477 | 3379359 |
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# Reformulations for MIQCPs: Products with 0-1 Variables

A quadratic term

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

can equivalently be replaced by

- an auxiliary variable $w$
- and the additional linear constraints

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

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

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Products of $n$ binary variables $\Rightarrow$ Pseudo-Boolean optimization

- ▷ linearize dynamically [Berthold et al., 2009b]

Tighter relaxations: E.g.,

- better handling of quadratic constraints: lift-and-project [Saxena et al., 2010], multiterm relaxations [Bao et al., 2009]
- convexification of trilinear $(x \cdot y \cdot z)$, quadrilinear $(w \cdot x \cdot y \cdot z)$, and multilinear forms: [Meyer and Floudas, 2004, Cafieri et al., 2010, Luedtke et al., 2010, Belotti et al., 2010]
- linear inequalities for orthogonal disjunctions and bilinear covering sets $(\sum_i a_i x_i y_i + b_i x_i + c_i y_i \geq r)$: [Tawarmalani et al., 2008]
- convexification of $n-1$–convex functions: [Jach et al., 2008]

# Further topics

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Nonlinear Integer Programming: [Hemmecke et al., 2009]

# LP/MIP based techniques for solving MINLPs

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