MINLP Solver Technology

Stefan Vigerske

GAMS

10 March 2015

Outline

Solvers

Linear Relaxation of Non-Convex terms

More Relaxations for Quadratic programs

Even More Cuts ...

Reformulation / Presolving

Bound Tightening

Branching

Primal Heuristics

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Deterministic Global Optimization Solvers for MINLP

ANTIGONE (**A**lgorithms for co**NT**inuous / **I**nteger **G**lobal **O**ptimization of **N**onlinear **E**quations)

- by R. Misener (Imperial) and C.A. Floudas (Princeton)
- originating from a solver for pooling problems
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- Misener and Floudas [2012a,b, 2014], Misener [2012]

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BARON (**B**ranch **A**nd **R**educe **O**ptimization **N**avigator)

- by N. Sahinidis (CMU) and M. Tawarmalani (Purdue)
- one of the first general purpose codes
- available as commercial solver in AIMMS and GAMS
- Tawarmalani and Sahinidis [2002, 2004, 2005]

Deterministic Global Optimization Solvers for MINLP

Couenne (**C**onvex **O**ver and **U**nder **EN**velopes for **N**onlinear **E**stimation)

- by P. Belotti (CMU, Clemson, now FICO)
- COIN-OR open source solver based on Bonmin (based on CBC and Ipopt)
- supports also trigonometric functions (sin, cos)
- available for AMPL and in GAMS and OS
- Belotti, Lee, Liberti, Margot, and Wächter [2009]

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LindoAPI

- by Y. Lin and L. Schrage (LINDO Systems, Inc.)
- supports many functions, incl. trigonometric (sin, cos)
- available as commercial solver within LINDO and GAMS
- Lin and Schrage [2009]

Deterministic Global Optimization Solvers for MINLP

SCIP (**S**olving **C**onstraint **I**nteger **P**rograms)

- by Zuse Institute Berlin, TU Darmstadt, ...
- part of a constraint integer programming framework
- free for academic use, available for AMPL and in GAMS
- Berthold, Gleixner, Heinz, and Vigerske [2012], Vigerske [2013]

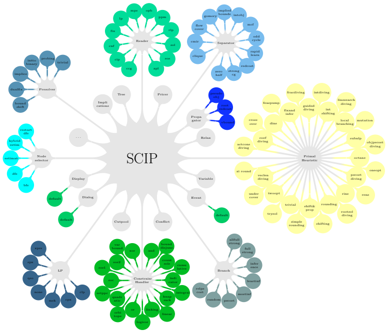
MIP
- LP relaxation
- cutting planes
- column generation

GO
- spatial branching

CP
- domain propagation

SAT
- conflict analysis
- periodic restarts

MIP, GO, CP, and SAT
- branch-and-bound



Upcoming Deterministic Global Solvers for MINLP

COCONUT (**CO**ntinuous **CON**straints – **U**pdating the **T**echnology)

- by A. Neumaier, H. Schichl, E. Monfroy (Vienna), et.al.
- rigorous calculations via interval arithmetics, thus avoiding floating point roundoff errors
- still in development, no stable release so far
- Neumaier [2004], Bliek et al. [2001]

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MINOTAUR (**M**ixed-**I**nteger **N**onconvex **O**ptimization **T**oolbox – **A**lgorithms, **U**nderestimators, **R**elaxations)

- by A. Mahajan, S. Leyffer, J. Linderoth, J. Luedtke, T. Munson, et.al. (Argonne, Wisconsin-Madison, IIT Bombay)
- open source with AMPL interface
- branch-and-bound with NLP relaxation (or its QP approximation); facilities to handle and manipulate algebraic expression are in place
- Mahajan and Munson [2010], Mahajan et al. [2012]

Further MINLP Solvers

Mixed-Integer Quadratic / Second Order Cone:

- CPLEX (IBM): AIMMS, AMPL, GAMS
- GUROBI: AIMMS, AMPL, GAMS
- MOSEK: AIMMS, AMPL, GAMS
- XPRESS (FICO): AIMMS, AMPL, GAMS

Convex MINLP:

- AlphaECP (Westerlund et.al., Åbo Akademi University, Finland): GAMS
- AOA (Paragon Decision Technology): AIMMS
- Bonmin (Bonami et.al., COIN-OR): AMPL, GAMS
- DICOPT (Grossmann et.al., CMU): GAMS
- FilMINT (Leyffer et.al., Argonne; Linderoth et.al., Lehigh): AMPL
- Knitro (Ziena Optimization): AIMMS, AMPL, GAMS
- SBB (ARKI Consulting): GAMS
- XPRESS-SLP (FICO)

Stochastic Search:

- LocalSolver (Innovation 24): GAMS
- OQNLP (OptTek Systems, Optimal Methods): GAMS

MINLP Solver Survey: Bussieck and Vigerske [2010]

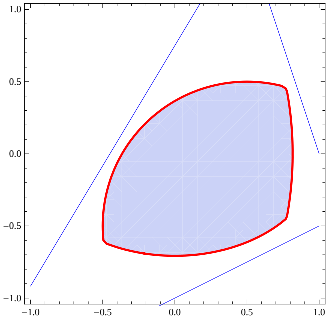
Outline

LP Relaxation of (MI)NLP

Convex Constraints $g(x) \leq 0$:

- Take some point x^* and linearize in x^*:

$$g(x^*) + \nabla g(x^*)(x - x^*) \leq 0$$



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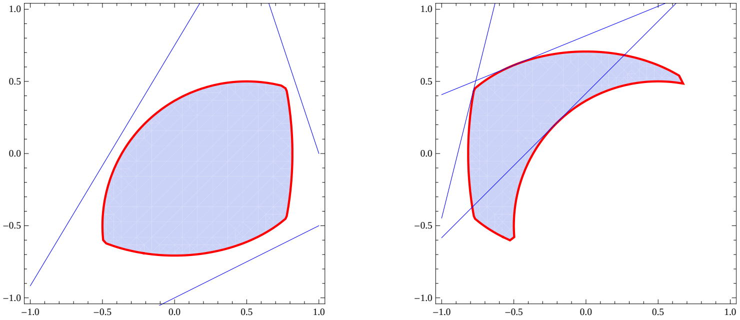
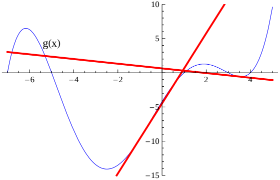
- may not work if $g_j(\cdot)$ is nonconvex !



Convex Underestimators

Inequalities $g(x^*) + \nabla g(x^*)^T (x - x^*) \leq 0$ may not be valid!



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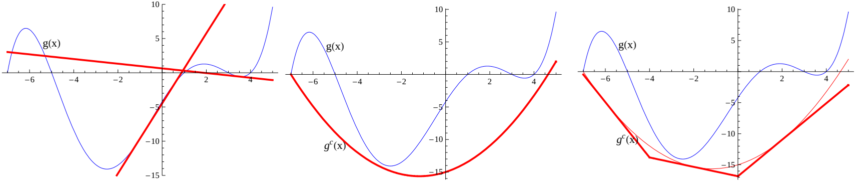
Inequalities $g(x^*) + \nabla g(x^*)^T (x - x^*) \le 0$ may not be valid!

- use convex underestimator: convex and below $g(x)$ for all $x \in [\underline{x}, \overline{x}]$
- introduces convexification gap



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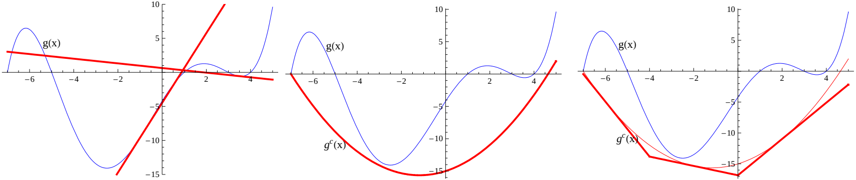
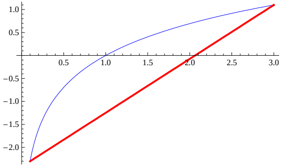
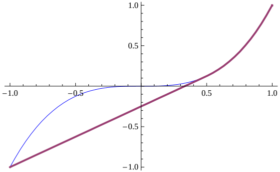


- convex envelopes (largest convex function that underestimates some $g(x)$) are difficult to find in general
- but are known for several simple cases:

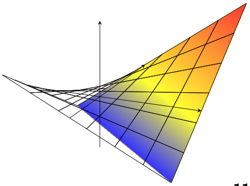
concave functions



$x \mapsto x^k$, $k \in 2\mathbb{Z} + 1$



$x \cdot y$

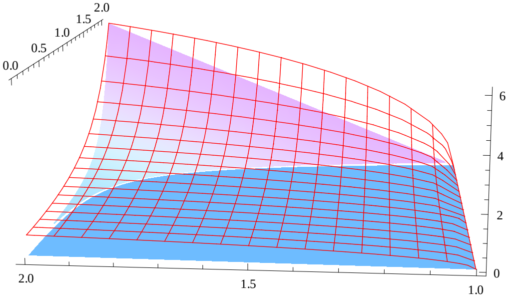


Reformulation of factorable functions

- for general factorable functions (recursive sum of products of univariate functions), reformulate into simple cases by introducing new variables and equations

Example:

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



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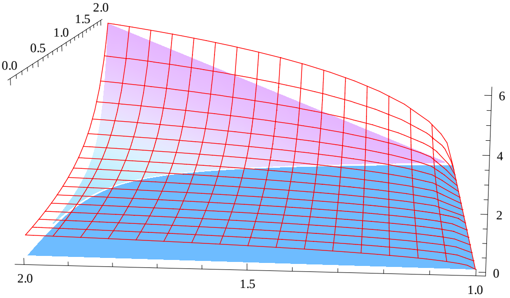
Reformulation:

$$g = \sqrt{y_1}$$
$$y_1 = y_2 y_3$$
$$y_2 = \exp(y_4)$$
$$y_3 = \ln(x_2)$$
$$y_4 = x_1^2$$



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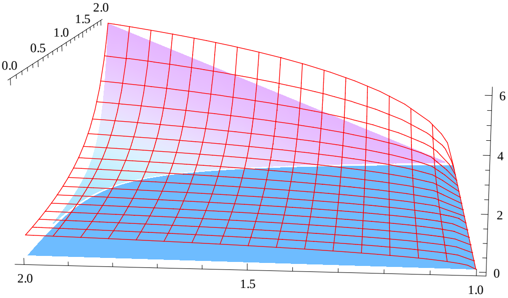

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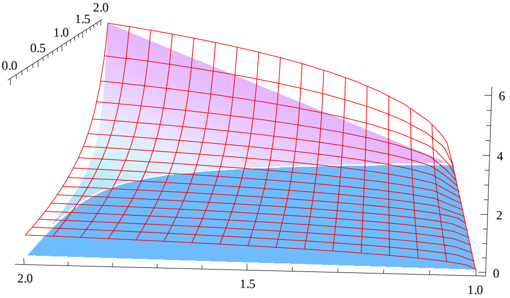


Convex relaxation:

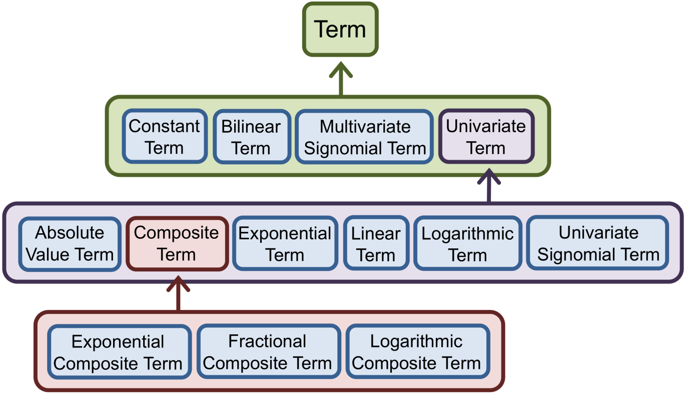
$$\sqrt{\underline{y_1}} + \frac{y_1 - \underline{y_1}}{\sqrt{\overline{y_1}} + \sqrt{\underline{y_1}}} \le g \le \sqrt{y_1}; \quad \ln \underline{x_2} + (x_2 - \underline{x_2})\frac{\ln \overline{x_2} - \ln \underline{x_2}}{\overline{x_2} - \underline{x_2}} \le y_3 \le \ln(x_2)$$

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

Basic Terms

The algebraic expressions that are not broken up further (i.e., convex & concave estimators are known) depends on the solver.

Example: Classification of terms in ANTIGONE:



[Misener and Floudas, 2014]

Implications of Expression Analysis Approach

- Deterministic global optimization algorithms need to know the algebraic expressions that the equations consist of, so they know how to convexify.

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- Deterministic global optimization algorithms need to know the algebraic expressions that the equations consist of, so they know how to convexify.
- Therefor, not all function types are supported by any deterministic global solver, e.g.,
  - ANTIGONE, BARON, and SCIP do not support trigonometric functions.
  - Couenne does not support max or min.
  - No deterministic global solver support external functions that are given by routines for point-wise evaluation of function and derivatives.

Bound your Variables!

- To construct convex underestimators, typically variable bounds are required. Otherwise, the solver may "guess" some bounds (ANTIGONE, BARON) or is not guarantee to finish within finite time (Couenne, SCIP).
- Example: $\min x \cdot y$

```
BARON version 12.3.3. Built: LNX-64 Fri Jun 14 08:14:38 EDT 2013
Preprocessing found feasible solution with value -.732842950994E+15
[...]
User did not provide appropriate variable bounds.
Some model expressions are unbounded.
We may not be able to guarantee globality.
Number of missing variable or expression bounds =      4
Number of variable or expression bounds autoset =      4
[...]
                       *** Normal Completion ***
        *** User did not provide appropriate variable bounds ***
              *** Globality is therefore not guaranteed ***

**** SOLVER STATUS     1 Normal Completion
**** MODEL STATUS      2 Locally Optimal
**** OBJECTIVE VALUE   -732842956409000.0000
```

- tighter variable bounds $\Rightarrow$ tighter relaxations

Fractional Terms

Convex underestimator of ${}^{x}/_{y}$ for $x, y \geq 0$ by Zamora and Grossmann [1998]:

$$\frac{x}{y} \geq \frac{1}{y} \left(\frac{x + \sqrt{\underline{x}\overline{x}}}{\sqrt{\underline{x}} + \sqrt{\overline{x}}} \right)^2,$$

(convex envelope if $\underline{y} = 0$, $\overline{y} = \infty$ [Tawarmalani and Sahinidis, 2001])

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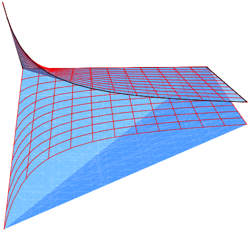
For $\overline{y} < \infty$, convex and concave envelopes are

$$\frac{\overline{x}-x}{\overline{x}-\underline{x}}\frac{\underline{x}}{\max\left(\underline{y}, \frac{\overline{y}-y}{\overline{x}-x}(\underline{x}-x)+y, \frac{y\sqrt{\underline{x}}(\overline{x}-\underline{x})}{(\overline{x}-x)\sqrt{\underline{x}}+(x-\underline{x})\sqrt{\overline{x}}}\right)}$$
$$+\frac{x-\underline{x}}{\overline{x}-\underline{x}}\frac{\overline{x}}{\min\left(\overline{y}, \frac{y-\underline{y}}{x-\underline{x}}(\overline{x}-x)+y, \frac{y\sqrt{\overline{x}}(\overline{x}-\underline{x})}{(\overline{x}-x)\sqrt{\underline{x}}+(x-\underline{x})\sqrt{\overline{x}}}\right)} \leq \frac{x}{y},$$

$$\frac{1}{\underline{y}\overline{y}}\min\{\overline{y}x-\underline{x}y+\underline{x}\underline{y}, \underline{y}x-\overline{x}y+\overline{x}\overline{y}\} \geq \frac{x}{y}$$



[Zamora and Grossmann, 1999, Tawarmalani and Sahinidis, 2002, Jach et al., 2008]

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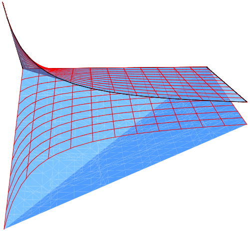

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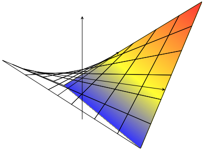
More formulas for $\frac{x}{y}$ with $\underline{x} < 0 < \overline{x}$, $\frac{ax+by}{cx+dy}$, $\frac{f(x)}{y}$ with f univariate concave, ... [Tawarmalani and Sahinidis, 2001, 2002].

Multilinear Terms

Bilinear $x \cdot y$:

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



[McCormick, 1976, Al-Khayyal and Falk, 1983]

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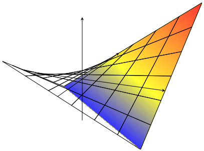

[McCormick, 1976, Al-Khayyal and Falk, 1983]

Trilinear $x \cdot y \cdot z$:

- Similar formulas by recursion, considering $(x \cdot y) \cdot z$, $x \cdot (y \cdot z)$, and $(x \cdot z) \cdot y$
  $\Rightarrow$ 18 inequalities for convex underestimator [Meyer and Floudas, 2004]

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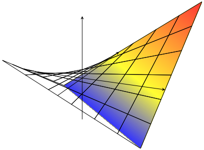

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- if mixed signs, e.g., $\underline{x} < 0 < \overline{x}$, recursion may not provide the convex envelope
- Meyer and Floudas [2004] derive the facets of the envelopes: for convex envelope, distinguish 9 cases, each giving 5-6 linear inequalities
- implemented in Couenne

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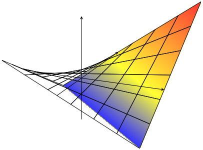

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Quadrilinear $u \cdot v \cdot w \cdot x$:

- Cafieri et al. [2010]: apply formulas for bilinear and trilinear to groupings $((u \cdot v) \cdot w) \cdot x$, $(u \cdot v) \cdot (w \cdot x)$, $(u \cdot v \cdot w) \cdot x$, $(u \cdot v) \cdot w \cdot x$ and compare strength numerically

Multilinear Terms

Let $$f(x) = \sum_{I \in \mathcal{I}} a_I \prod_{i \in I} x_i \qquad (I \subseteq \{1, \dots, n\}) \qquad \text{with bounds } x \in [\underline{x}, \overline{x}].$$

- Luedtke et al. [2012]: compare strength of relaxation from recursive application of McCormick with convex envelope

Multilinear Terms

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$$= \max_{a \in \mathbb{R}^n, b \in \mathbb{R}} \{ a^T x + b \;:\; a^T v^p + b \leq f(v^p)\, \forall p \}, \qquad \text{(D)}$$

where $\{v^p : p = 1, \ldots, 2^n\} = \text{vert}([\underline{x}, \overline{x}])$ are the vertices of the box $[\underline{x}, \overline{x}]$.

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- Bao et al. [2009] (BARON): for quadratic multilinear functions, solve (C) by column generation

Edge-Concave Functions

Definition [Tardella, 2004]: A function $f : \mathbb{R}^n \to \mathbb{R}$ is edge-concave on the box $[\underline{x}, \overline{x}]$, if it is concave on all segments that are parallel on an edge of $[\underline{x}, \overline{x}]$.

Tardella [1988/89]: If f is twice continuously differentiable, then it is

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A quadratic function

$$x^T Q x = \sum_{i \leq j} Q_{i,j} x_i x_j$$

is edge-concave if $Q_{i,i} \leq 0$ for all i

Cuts from Edge-Concave Functions ($n = 3$)

Meyer and Floudas [2005], Tardella [2008]: Some facets of the convex envelope of

$$\underbrace{Q_{1,1}}_{\leq 0} x_1^2 + \underbrace{Q_{2,2}}_{\leq 0} x_2^2 + \underbrace{Q_{3,3}}_{\leq 0} x_3^2 + \underbrace{Q_{1,2}}_{\neq 0} x_1 x_2 + \underbrace{Q_{1,3}}_{\neq 0} x_1 x_3 + \underbrace{Q_{2,3}}_{\neq 0} x_2 x_3,$$

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GLOMIQO 1.0 (predecessor of ANTIGONE) [Misener and Floudas, 2012a]:

- group quadratic terms in constraints into sums of three-dimensional edge-concave and convex functions
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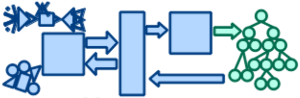
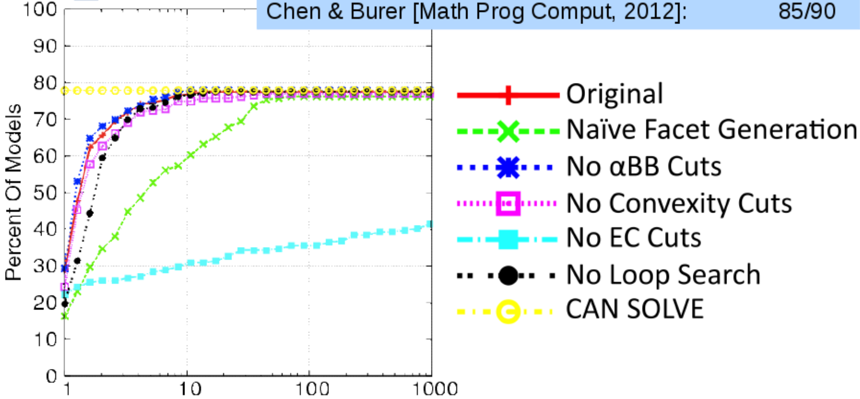
GloMIQO 2.0 / ANTIGONE [Misener, 2012]:

- reduced complexity approach based on Meyer and Floudas [2005] (exploiting dominance relations)
- complexity scales by $n!$ instead of $\binom{2^n}{n+1}$

ANTIGONE: Dynamically Adding Cuts



BoxQP: 54/54; 72/90
Vandenbussche & Nemhauser [Math Prog, 2005]: 53/54
Burer & Vandenbussche [Math Prog, 2008]: 78/90
Chen & Burer [Math Prog Comput, 2012]: 85/90



Bivariate Terms

Given $f(x,y) \in C^2(\mathbb{R}^2,\mathbb{R})$, $x \in [\underline{x},\overline{x}]$, $y \in [\underline{y},\overline{y}]$, with fixed convexity behaviour ($\operatorname{sign}\nabla^2_{x,x} f$, $\operatorname{sign}\nabla^2_{y,y} f$, $\operatorname{sign}\nabla^2_{x,y} f$, $\operatorname{sign}\det\nabla^2 f$ are constant on $[\underline{x},\overline{x}] \times [\underline{y},\overline{y}]$).

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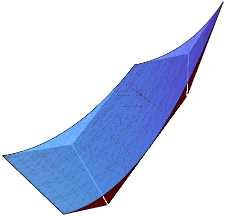
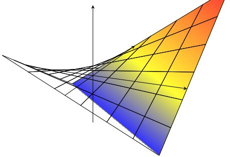
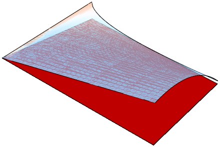
Convexity behaviour of f	Convex Envelope
jointly convex	f itself
concave in x, concave in y	vertex-polyhedral, thus McCormick [1976]
convex in x, concave in y (or other way around)	Tawarmalani and Sahinidis [2001] Locatelli and Schoen [2014], Locatelli [2010]
convex in x, convex in y, indefinite	Jach, Michaels, and Weismantel [2008] Locatelli and Schoen [2014], Locatelli [2010]



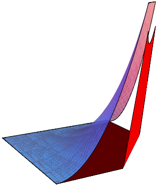
$f(x,y) = x^2/y$



$f(x,y) = xy$



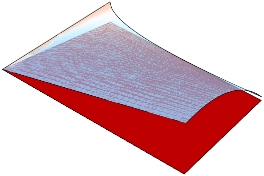
$f(x,y) = -\sqrt{x}y^2$



$f(x,y) = x^2y^2$

$f(x, y)$ convex in x and concave in y

Convex envelope in $(x^0, y^0) \in \operatorname{int}([\underline{x}, \overline{x}] \times [\underline{y}, \overline{y}])$ given by



$$\begin{aligned} \operatorname{vex}[f](x^0, y^0) := \min\ & t f(r, \underline{y}) + (1-t) f(s, \overline{y}) \\ \text{s.t. } & \begin{pmatrix} x^0 \\ y^0 \end{pmatrix} = t \begin{pmatrix} r \\ \underline{y} \end{pmatrix} + (1-t) \begin{pmatrix} s \\ \overline{y} \end{pmatrix} \\ & t \in [0,1], \quad r, s \in [\underline{x}, \overline{x}] \end{aligned}$$

[Tawarmalani and Sahinidis, 2001, Jach et al., 2008]

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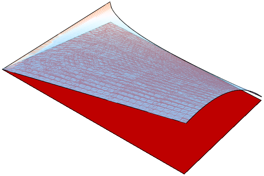

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Using $t = \frac{\overline{y} - y^0}{\overline{y} - \underline{y}}$, $r(s) = \frac{\overline{y} - \underline{y}}{\overline{y} - y^0} x^0 - \frac{y^0 - \underline{y}}{\overline{y} - y^0} s$, this simplifies to

$$\text{vex}[f](x^0, y^0) = \min_{s \in [\underline{s}, \overline{s}]} \frac{\overline{y} - y^0}{\overline{y} - \underline{y}} f\left(\frac{\overline{y} - \underline{y}}{\overline{y} - y^0} x^0 - \frac{y^0 - \underline{y}}{\overline{y} - y^0} s, \underline{y} \right) + \frac{y^0 - \underline{y}}{\overline{y} - \underline{y}} f(s, \overline{y})$$

$\Rightarrow$ univariate convex optimization problem

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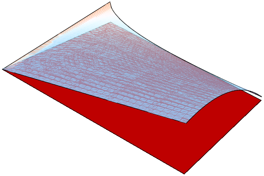

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$\Rightarrow$ univariate convex optimization problem

Maximally touching hyperplane on graph of $\operatorname{vex}[f]$ at (x^0, y^0) is given by

$$\begin{pmatrix} x^0 \\ y^0 \\ \operatorname{vex}[f](x^0, y^0) \end{pmatrix} + \mathbb{R} \begin{pmatrix} s^* - r^* \\ \overline{y} - \underline{y} \\ f(s^*, \overline{y}) - f(r^*, \underline{y}) \end{pmatrix} + \mathbb{R} \begin{pmatrix} 1 \\ 0 \\ \frac{\partial f}{\partial x}(\hat{x}, \hat{y}) \end{pmatrix}, \ (\hat{x}, \hat{y}) = (r^*, \underline{y}) \text{ or } (s^*, \overline{y}).$$

Ballerstein et al. [2013]: implementation in SCIP

(so far, classification of convexity behavior only for $f(x,y) = x^p y^q$, $x, y \geq 0$)

Outline

α-Underestimators [Androulakis et al., 1995, Adjiman and Floudas, 1996]

Consider a function $x^T A x + b^T x$ with $A \not\succeq 0$.

Let $\alpha \in \mathbb{R}^n$ be such that $A - \mathrm{diag}(\alpha) \succeq 0$. Then

$$x^T A x + b^T x + (\overline{x} - x)^T \mathrm{diag}(\alpha)(x - \underline{x})$$

is a convex underestimator of $x^T A x + b^T x$ w.r.t. the box $[\underline{x}, \overline{x}]$.

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- available in ANTIGONE (in a modified form, see Misener [2012]) and Couenne (off by default)
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- underestimator is exact for $x_i \in \{\underline{x}_i, \overline{x}_i\}$
- thus, if x is a vector of binary variables ($x_i^2 = x_i$), then

$$x^T Ax + b^T x = x^T (A - \text{diag}(\alpha))x + (b + \text{diag}(\alpha))^T x$$

for $x \in \{0, 1\}^n$ and $A - \text{diag}(\alpha) \succeq 0$. $\Rightarrow$ used in CPLEX

Eigenvalue Reformulation

Consider a function $x^T A x + b^T x$ with $A \not\succeq 0$.

- Let $\lambda_1, \ldots, \lambda_n$ be eigenvalues of A and $v_1, \ldots, v_n$ be corresp. eigenvectors.

$$\Rightarrow \qquad x^T A x + b^T x + c = \sum_{i=1}^{n} \lambda_i (v_i^T x)^2 + b^T x + c. \tag{E}$$

- introducing auxiliary variables $z_i = v_i^T x$, function becomes separable:

$$\sum_{i=1}^{n} \lambda_i z_i^2 + b^T x + c$$

- underestimate concave functions $z_i \mapsto \lambda_i z_i^2$, $\lambda_i < 0$, as known

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- underestimate concave functions $z_i \mapsto \lambda_i z_i^2$, $\lambda_i < 0$, as known
- one of the methods for nonconvex QP in CPLEX (keeps convex $\lambda_i z_i^2$ in objective and solves relaxation by QP simplex)
- ANTIGONE can make use of representation (E) to compute cuts in the spirit of Saxena et al. [2011] [Misener and Floudas, 2012b]

Reformulation Linearization Technique (RLT)

Consider the QCQP

$$
\begin{aligned}
\min\ & x^T Q_0 x + b_0^T x && && \text{(quadratic)} \\
\text{s.t. } & x^T Q_k x + b_k^T x \le c_k && k = 1, \ldots, q && \text{(quadratic)} \\
& Ax \le b && && \text{(linear)} \\
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Introduce new variables $X_{i,j} = x_i x_j$:

$$
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\min\ & \langle Q_0, X \rangle + b_0^T x && && \text{(linear)} \\
\text{s.t. } & \langle Q_k, X \rangle + b_k^T x \le c_k && k = 1, \ldots, q && \text{(linear)} \\
& Ax \le b && && \text{(linear)} \\
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Adams and Sherali [1986], Sherali and Alameddine [1992], Sherali and Adams [1999]:

- relax $X = xx^T$ by linear inequalities that are derived from multiplications of pairs of linear constraints

RLT: Multiplying Bound Constraints

Multiplying bounds $\underline{x}_i \leq x_i \leq \overline{x}_j$ and $\underline{x}_j \leq x_j \leq \overline{x}_j$ yields

$$(x_i - \underline{x}_i)(x_j - \underline{x}_j) \geq 0$$
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RLT: Multiplying Bound Constraints

Multiplying bounds $\underline{x}_i \leq x_i \leq \overline{x}_j$ and $\underline{x}_j \leq x_j \leq \overline{x}_j$ and using $X_{i,j} = x_i x_j$ yields

$$
\begin{aligned}
(x_i - \underline{x}_i)(x_j - \underline{x}_j) \geq 0 \quad &\Rightarrow \quad X_{i,j} \geq \underline{x}_i x_j + \underline{x}_j x_i - \underline{x}_i \underline{x}_j \\
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Multiplying bounds $\underline{x}_i \leq x_i \leq \overline{x}_j$ and $\underline{x}_j \leq x_j \leq \overline{x}_j$ and using $X_{i,j} = x_i x_j$ yields

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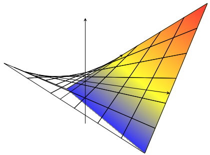

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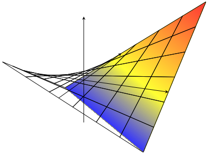

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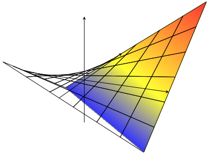

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- these inequalities are used by all solvers
- not every solver introduces $X_{i,j}$ variables explicitly

RLT: Multiplying Bounds and Inequalities

Additional inequalities are derived by multiplying pairs of linear equations and bound constraints:

$$(A_\ell^T x - b_\ell)(x_j - \underline{x}_j) \geq 0 \quad \Rightarrow \quad \sum_{i=1}^{n} A_{\ell,i} x_i (x_j - \underline{x}_j) - b_\ell (x_j - \underline{x}_j) \geq 0$$

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  (close to bilinear term elimination of Liberti and Pantelides [2006])

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  (close to bilinear term elimination of Liberti and Pantelides [2006])
- in all cases, consider only products that do not add new nonlinear terms
  (avoid $X_{i,j}$ without corresponding $x_i x_j$)
- learn useful RLT cuts in the first levels of branch-and-bound

RLT: Give your solver ~~a hand~~ an equation.

Misener and Floudas [2012b]:

- *As a final observation with respect to generating RLT equations, notice that a modeler will significantly improve the performance of GloMIQO by writing linear constraints that can be multiplied together without increasing the number of nonlinear terms.*

$\Rightarrow$ RLT is an example where adding redundant constraints can help (recall Jeff's slides on the pooling problem).

Semidefinite Programming (SDP) Relaxation

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\min\ & x^T Q_0 x + b_0^T x \\
\text{s.t. } & x^T Q_k x + b_k^T x \le c_k \\
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- relaxing $X - xx^T = 0$ to $X - xx^T \succeq 0$, which is equivalent to

$$\tilde{X} := \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0,$$

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  yields a semidefinite programming relaxation
- SDP is computationally demanding, so approximate by linear inequalities
  Sherali and Fraticelli [2002]:
  for $\tilde{X}^* \not\succeq 0$ compute eigenvector v with eigenvalue $\lambda < 0$, then

$$\langle v, \tilde{X} v \rangle \geq 0$$

  is a valid cut that cuts off $\tilde{X}^*$
- available in Couenne and Lindo API (non-default)
- Qualizza et al. [2012] (Couenne): sparsify cut by setting entries of v to 0
- Saxena et al. [2011]: project into x-variables space (no $X_{i,j}$ variables needed)

SDP vs RLT vs α-BB

Anstreicher [2009]:

- the SDP relaxation does not dominate the RLT relaxation
- the RLT relaxation does not dominate the SDP relaxation
- combining both relaxations can produce substantially better bounds

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Anstreicher [2012]:

- the SDP relaxation dominates the α-BB underestimators

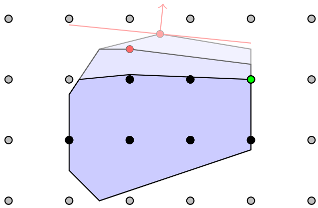
Outline

More Cutting Planes for MINLP

MIP $\subset$ MINLP, so don't forget about the MIP cuts:

- Gomory
- Mixed-Integer Rounding
- Flow Cover
- ...

Available in ANTIGONE (via CPLEX), BARON, Couenne (off by default), SCIP, and Lindo API.



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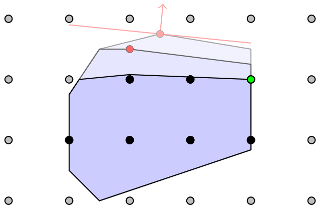

Disjunctive Programming Cuts:

- given the (tightened) LP relaxations after branching on a variable, compute a cut that is valid for the union of both relaxations
- apply during strong branching
- available in FilMINT and Couenne [Kilinç et al., 2010, Belotti, 2012]
- see also Bonami, Linderoth, and Lodi [2012] for a review

Outline

Convexity Detection

Analyze the Hessian:

$$f(x) \text{ convex on } [\underline{x}, \overline{x}] \quad \Leftrightarrow \quad \nabla^2 f(x) \succeq 0 \quad \forall x \in [\underline{x}, \overline{x}]$$

- $f(x)$ is quadratic $\Rightarrow$ $\nabla^2 f(x)$ constant $\Rightarrow$ compute spectrum numerically
- done by ANTIGONE, Couenne (off by default), BARON, SCIP
- general $f \in C^2$ $\Rightarrow$ estimate eigenvalues of Interval-Hessian [Nenov et al., 2004]

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Analyze the Algebraic Expression:

$$f(x) \text{ convex} \Rightarrow a \cdot f(x) \begin{cases} \text{convex}, & a \geq 0 \\ \text{concave}, & a \leq 0 \end{cases}$$

$$f(x), g(x) \text{ convex} \Rightarrow f(x) + g(x) \text{ convex}$$

$$f(x) \text{ concave} \Rightarrow \log(f(x)) \text{ concave}$$

$$f(x) = \prod_i x_i^{e_i}, x_i \geq 0 \Rightarrow f(x) \begin{cases} \text{convex}, & e_i \leq 0 \;\forall i \\ \text{convex}, & \exists j : e_i \leq 0 \;\forall i \neq j;\; \sum_i e_i \geq 1 \\ \text{concave}, & e_i \geq 0 \;\forall i;\; \sum_i e_i \leq 1 \end{cases}$$

Available in ANTIGONE, BARON, and SCIP.

[Maranas and Floudas, 1995, Bao, 2007, Fourer et al., 2009, Vigerske, 2013]

Second Order Cones (SOC)

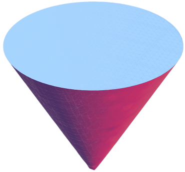
Consider a constraint $\quad x^T A x + b^T x \leq c.$

- if A has only one negative eigenvalue, it may be reformulated as a second-order cone constraint [Mahajan and Munson, 2010], e.g.,

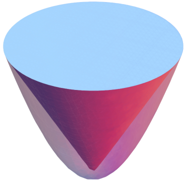
$$\sum_{k=1}^{N} x_k^2 - x_{N+1}^2 \leq 0, x_{N+1} \geq 0 \qquad \Leftrightarrow \qquad \sqrt{\sum_{k=1}^{N} x_k^2} \leq x_{N+1}$$

- $\sqrt{\sum_{k=1}^{N} x_k^2}$ is a convex term that can easily be linearized
- BARON and SCIP recognize "obvious" SOCs $\left(\sum_{k=1}^{N} (\alpha_k x_k)^2 - (\alpha_{N+1} x_{N+1})^2 \leq 0\right)$

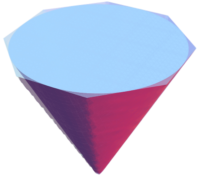
Example: $x^2 + y^2 - z^2 \leq 0$ in $[-1, 1] \times [-1, 1] \times [0, 1]$



feasible region



not recognizing SOC



recognizing SOC

(initial relaxation)

More Presole

- Products with binary variables can be linearized:

$$x \cdot \sum_{k=1}^{N} a_k y_k \text{ with } x \in \{0,1\} \Leftrightarrow \begin{aligned} M^L x \leq & w \leq M^U x, \\ \sum_{k=1}^{N} a_k y_k - M^U(1-x) \leq & w \leq \sum_{k=1}^{N} a_k y_k - M^L(1-x), \end{aligned}$$

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

Implemented by Lindo API and SCIP.

$\Rightarrow$ Don't rewrite $x \cdot y$ as Big-M! – the solver may do it for you :-)

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- Liberti [2012], Liberti and Ostrowski [2014]: Automated symmetry detection and breaking for Couenne ("orbital branching", off by default)

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- MINOTAUR: Coefficient tightening for certain nonlinear constraints:

$$c(x) \leq b + M(1-y) \qquad y \in \{0,1\}, \quad 0 \leq x_i \leq \bar{x}_i y$$

$$\Rightarrow c(x) + (c(0) - b)y \leq c(0)$$

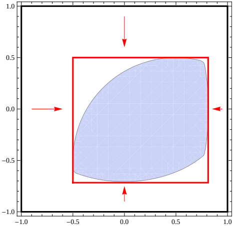
[Belotti, Kirches, Leyffer, Linderoth, Luedtke, and Mahajan, 2013]

Outline

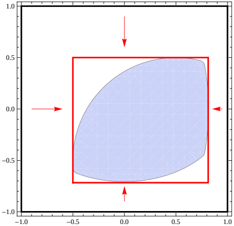
Bounds Tightening (Domain Propagation)

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



Bounds Tightening (Domain Propagation)



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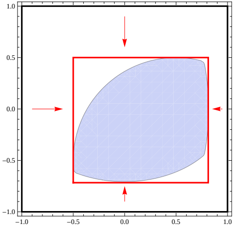

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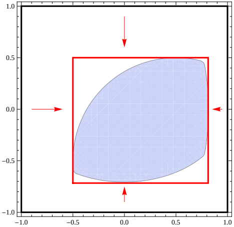

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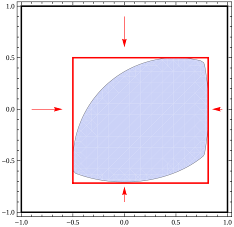

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Some techniques [Belotti et al., 2009]:

	Reduced Cost Bounds Tightening (cheap), same as in MIP
FBBT	Feasibility-Based Bounds Tightening (cheap)
ABT	Aggressive Feasibility-Based Bounds Tightening (expensive)
OBBT	Optimality/Optimization-Based Bounds Tightening (expensive)

FBBT for Linear Constraints

Feasibility-Based Bound Tightening for a linear constraint:

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

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

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Represent algebraic structure of problem in one directed acyclic graph:

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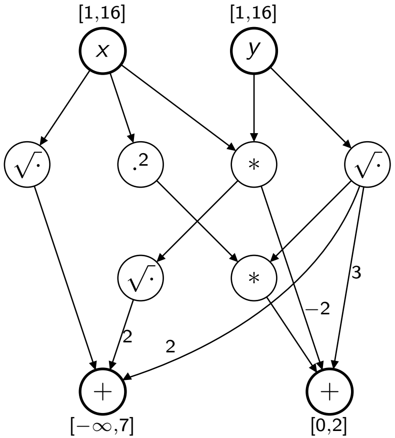
$$x, y \in [1, 16]$$



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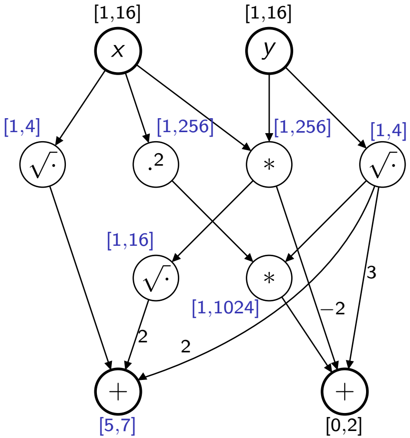

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- compute bounds on intermediate nodes (top-down)

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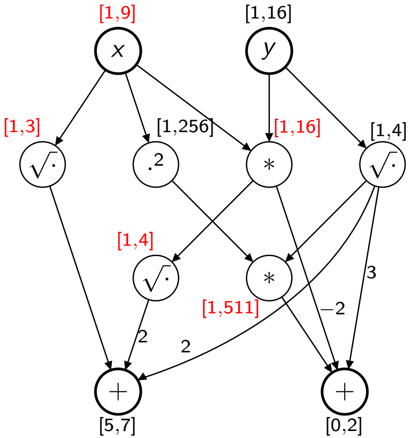
Backward propagation:

- reduce bounds using reverse operations (bottom-up)



Aggressive Bound Tightening (Probing)

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

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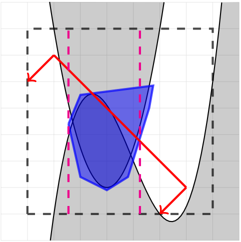
- Nannicini et al. [2011]:
  - instead of applying FBBT, do a limited branch-and-bound search on the reduced problem
  - use success of FBBT and a predictor to decide for which variables the method should be employed

Optimization-Based Bound Tightening (OBBT)

[Quesada and Grossmann, 1993, Maranas and Floudas, 1997, Smith and Pantelides, 1999, ...]

Given LP relaxation



$$\min\{c^T x : Ax \leq b, x \in [\underline{x}, \overline{x}]\},$$

solve for some variables x_k:

$$\min / \max \{x_k : Ax \leq b, c^T x \leq c^T x^*, x \in [\underline{x}, \overline{x}]\},$$

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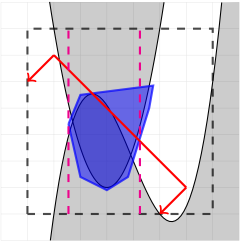

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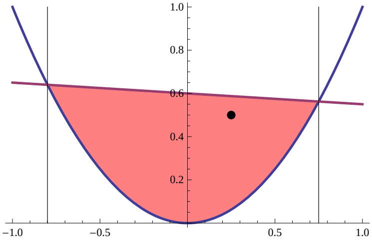
- Couenne: at nodes of depth ≤ 10, for deeper nodes with probability $2^{10-\text{depth}}$
- ANTIGONE: on nonlinear and binary variables as long as effective; if not effective for a node, disable for all child nodes
- SCIP: efficient implementation by Gleixner and Weltge [2013]:
  - bound filtering (exclude bounds with guaranteed fail)
  - bound grouping (heuristically search groups of bounds with likely success)
  - solve OBBT LPs only at root node, but learn new linear inequalities $x_k \geq r^T x + \mu \langle c, x^* \rangle + \lambda^T b$ from dual solution of LP

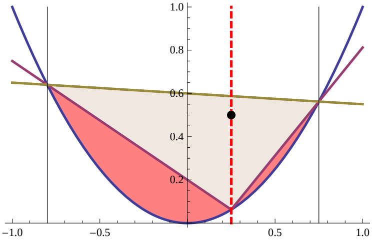
$\Rightarrow$ approximate OBBT during tree search

Outline

Spatial Branching

Branching on a nonlinear variable in a nonconvex term allows for tighter relaxations:





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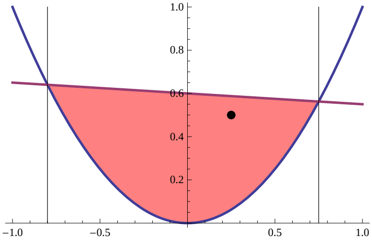

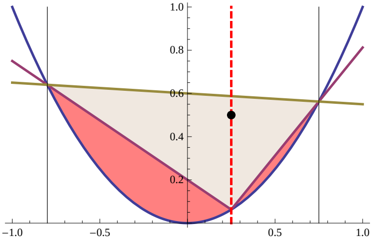

How to select the branching variable from a set of variable candidates?

Belotti, Lee, Liberti, Margot, and Wächter [2009]: adapt branching rules for discrete variables in MIP (most fractional, strong branching, pseudo costs, reliability branching) to continuous variables

Branching Rule: Most violated

"Most fractional" rule for integer variables:

- branch on variable with maximal fractional value in solution of LP relaxation ($\text{argmax}_{i \in I} \ \min\{\hat{x}_i - \lfloor \hat{x}_i \rfloor, \lceil \hat{x}_i \rceil - \hat{x}_i\}$)

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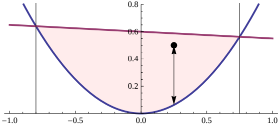
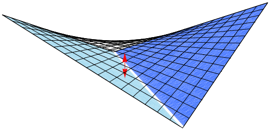
- for each variable, collect the "convexification gaps" for all nonconvex terms that involve this variable





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- available in Couenne and SCIP

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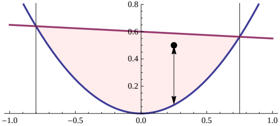

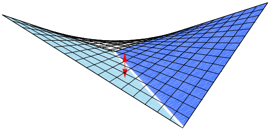

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"Violation transfer" [Tawarmalani and Sahinidis, 2004]:

- available in BARON

Branching Rule: Pseudo Costs

Integer variables x_i:

- when branching, memorize resulting change in lower bound relative to change in variable value due to branching ($\hat{x}_i - \lfloor \hat{x}_i \rfloor$, $\lceil \hat{x}_i \rceil - \hat{x}_i$)
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Continuous variables:

- branching does not result in immediate change of variable's value in LP

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- Belotti et al. [2009] proposed several alternatives for weighting the lower bound change:
  - variable infeasibility (analog to fractionality)
  - domain width after branching
- available in ANTIGONE and Couenne and used in SCIP

Branching Rules: Strong and 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
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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

⇒ initialization of pseudo costs by strong branching

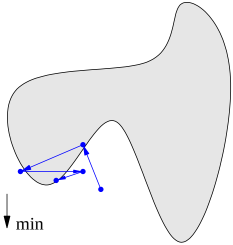
- used in ANTIGONE, BARON, and Couenne

Outline

Sub-NLP Heuristics

Given a solution satisfying all integrality constraints,

- fix all integer variables in the MINLP
- call an NLP solver to find a local solution to the remaining NLP



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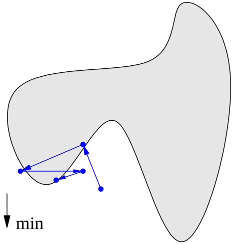

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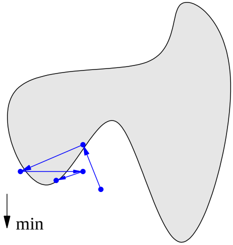

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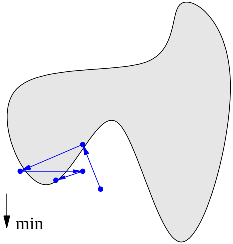


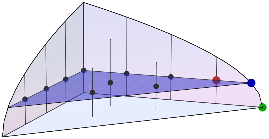
NLP-Diving:

- solve NLP relaxation, restrict bound on fractional variable, resolve NLP
- available in SCIP; QP-diving variant in MINOTAUR [Mahajan et al., 2012]

Sub-MIP / Sub-MINLP Heuristics

Berthold and Gleixner [2014]: “Undercover” (SCIP):

- Fix nonlinear variables, so problem becomes MIP (pass to SCIP)
- not always necessary to fix all nonlinear variables, e.g., consider $x \cdot y$
- find a minimal set of variables to fix by solving a Set Covering Problem



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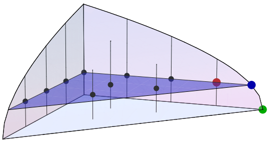
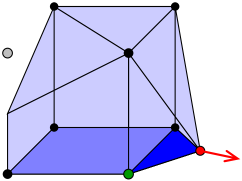


Berthold et al. [2011]: Large Neighborhood Search heuristics extended from MIP/CP to MINLP (SCIP):

- RENS [Berthold, 2014a]: fix integer variables with integral value in LP relaxation
- RINS, DINS, Crossover, Local Branching



Rounding Heuristics

Nannicini and Belotti [2012]: Couenne Iterative Rounding Heuristic (off by default):

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Berthold [2014b]: Couenne Feasibility Pump (off by default)

- alternately find feasible solutions to MIP and NLP relaxations
- solution of NLP relaxation is "rounded" to solution of MIP relaxation (by various methods trading solution quality with computational effort)
- solution of MIP relaxation is projected onto NLP relaxation (local search)
- various choices for objective functions and accuracy of MIP relaxation
- D'Ambrosio et al. [2010, 2012]: previous work on Feasibility Pump for nonconvex MINLP

End.

Thank you for your attention!

Consider contributing your MINLP instances to MINLPLib!

Some recent MINLP reviews:

- Burer and Letchford [2012]
- Belotti, Kirches, Leyffer, Linderoth, Luedtke, and Mahajan [2013]

Some recent books:

- Lee and Leyffer [2012]
- Locatelli and Schoen [2013]

Literature I

Warren P. Adams and Hanif D. Sherali. A tight linearization and an algorithm for zero-one quadratic programming problems. *Management Science*, 32(10):1274–1290, 1986. doi:10.1287/mnsc.32.10.1274.

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