MINLP Solver Technology

Stefan Vigerske

October 24, 2017

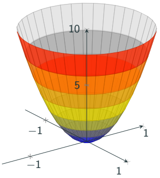
Outline

Introduction

Mixed-Integer Nonlinear Programs (MINLPs)

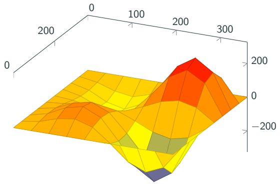
$$
\begin{aligned}
\min\ & c^{\mathsf{T}} x \\
\text{s.t. } & g_k(x) \le 0 && \forall k \in [m] \\
& x_i \in \mathbb{Z} && \forall i \in \mathcal{I} \subseteq [n] \\
& x_i \in [\ell_i, u_i] && \forall i \in [n]
\end{aligned}
$$

The functions $g_k \in C^1([\ell, u], \mathbb{R})$ can be



convex

or



nonconvex

Convex MINLP:

- Main difficulty: Integrality restrictions on variables
- Main challenge: Integrating techniques for MIP (branch-and-bound) and NLP (SQP, interior point, Kelley' cutting plane, ...)

Solving MINLPs

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General MINLP = Convex MINLP **plus** Global Optimization:

- Main difficulty: Nonconvex nonlinearities
- Main challenges:
  - Convexification of nonconvex nonlinearities
  - Reduction of convexification gap (spatial branch-and-bound)
  - Numerical robustness
  - Diversity of problem class: MINLP is "The mother of all determinstic optimization problems" (Jon Lee, 2008)

Solvers for Convex MINLP

solver	**citation**	**OA**	**NLP-BB**	**LP/NLP**
AlphaECP	Westerlund and Lundquist [2005], Lastusilta [2011]	ECP		
AOA	Roelofs and Bisschop [2017] (AIMMS)	✓		
Bonmin	Bonami, Biegler, Conn, Cornuéjols, Grossmann, Laird, Lee, Lodi, Margot, Sawaya, and Wächter [2008]	✓	✓	✓
DICOPT	Kocis and Grossmann [1989]	✓		
FilMINT	Abhishek, Leyffer, and Linderoth [2010]			✓
Knitro	Byrd, Nocedal, and Waltz [2006]		✓	
MINLPBB	Leyffer [1998]		✓	
MINOTAUR	Mahajan, Leyffer, and Munson [2009]		(✓)	
SBB	Bussieck and Drud [2001]		✓	
XPRESS-SLP	FICO [2008]	ECP	✓	
⋮				

- can often work as heuristic for nonconvex MINLP

Deterministic:

solver	1st ver.	citation
αBB	1995	Adjiman, Androulakis, and Floudas [1998a]
BARON	1996	Sahinidis [1996], Tawarmalani and Sahinidis [2005]
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SCIP	2012	Achterberg [2009], Vigerske and Gleixner [2017], Maher, Fischer, Gally, Gamrath, Gleixner, Gottwald, Hendel, Koch, Lübbecke, Miltenberger, Müller, Pfetsch, Puchert, Rehfeldt, Schenker, Schwarz, Serrano, Shinano, Weninger, Witt, and Witzig [2017]
ANTIGONE	2013	Misener and Floudas [2014]

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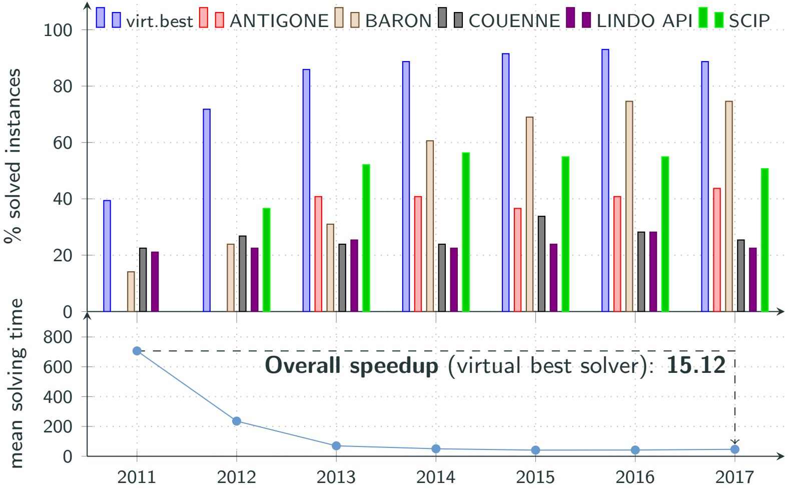
Main restriction: algebraic structure of problem must be available (see later)

Interval-Arithmetic based: avoid round-off errors, typically NLP only, e.g., COCONUT [Neumaier, 2001], Ibex, . . .

Stochastic search: LocalSolver, OQNLP [Ugray, Lasdon, Plummer, Glover, Kelly, and Martí, 2007], . . .

Global MINLP Solver Progress: # Solved Instances and Solving Time



- 71 "non-trivial solvable" instances from MINLPLib
- time limit: 1800 seconds, gap limit: 1e-6

date	ANTIGONE	BARON	COUENNE	LINDO API	SCIP
08/2011	–	**9.3**.1	**0.3**	**6.1**.1.588	–
11/2012	–	**11.5**.2	0.4	7.0.1.497	2.1.2
07/2013	**1.1**	**12.3**.3	0.4	**8.0**.1283.385	3.0
09/2014	1.1	**14.0**.3	0.4	8.0.1694.550	**3.1**
11/2015	1.1	**15.9**.22	**0.5**	9.0.2120.225	**3.2**
09/2016	1.1	**16.8**.24	0.5	9.0.2217.293	3.2
08/2017	1.1	**17.8**.7	0.5	**11.0**.3742.269	**4.0**

Fundamental Methods

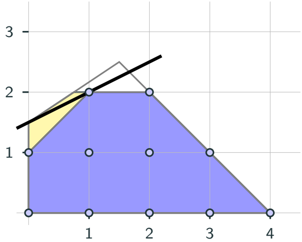
Fundamental Methods

Recap: Mixed-Integer Linear Programming

For mixed-integer linear programs (MIP), that is,

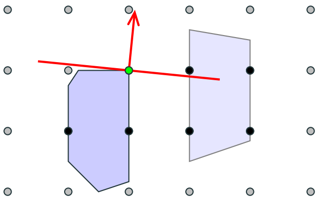
$$\begin{aligned} &\min c^{\mathsf{T}} x, \\ &\text{s.t. } Ax \le b, \\ &\quad x_i \in \mathbb{Z}, \quad i \in \mathcal{I}, \end{aligned}$$

the dominant method of **Branch & Cut** combines



cutting planes
[Gomory, 1958]

&

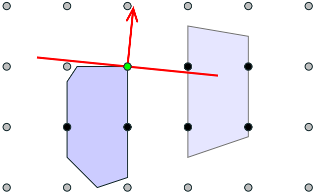


branch-and-bound
[Land and Doig, 1960]

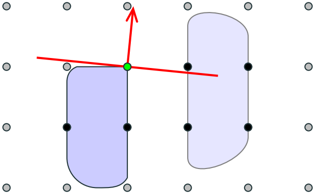
Fundamental Methods

Convex MINLP

NLP-based Branch & Bound (NLP-BB)



$\Rightarrow$



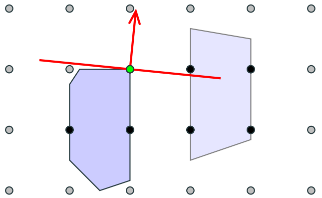
MIP branch-and-bound
[Land and Doig, 1960]

MINLP branch-and-bound
[Leyffer, 1993]

Bounding: Solve convex NLP relaxation obtained by dropping integrality requirements.

Branching: Subdivide problem along variables x_i, $i \in \mathcal{I}$, that take fractional value in NLP solution.

NLP-based Branch & Bound (NLP-BB)



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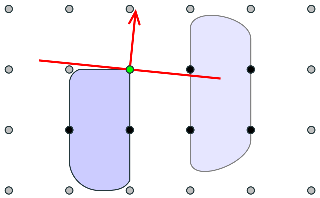

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Bounding: Solve convex NLP relaxation obtained by dropping integrality requirements.

Branching: Subdivide problem along variables x_i, $i \in \mathcal{I}$, that take fractional value in NLP solution.

- However: Robustness and Warmstarting-capability of NLP solvers not as good as for LP solvers (simplex alg.)

Reduce Convex MINLP to MIP

Assume all functions $g_k(\cdot)$ of MINLP are convex on $[\ell, u]$.

Duran and Grossmann [1986]: MINLP and the following MIP have the same optimal solutions

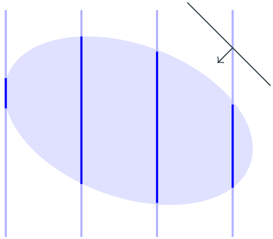
$$\begin{aligned} \min\ & c^\top x, \\ \text{s.t. } & g_k(\hat{x}) + \nabla g_k(\hat{x})^\top (x - \hat{x}) \leq 0, \\ & \quad k \in [m], \quad \hat{x} \in R, \\ & x_i \in \mathbb{Z}, \quad i \in \mathcal{I}, \\ & x \in [\ell, u], \end{aligned}$$

where $\hat{x} \in R$ are the solutions of the NLP subproblems obtained from MINLP by applying any possible fixing for $x_{\mathcal{I}}$, i.e.,

$$\min c^\top x \text{ s.t. } g(x) \leq 0, x \in [\ell, u], x_I \text{ fixed.}$$

Example:

$$\begin{aligned} \min\ & x + y \\ \text{s.t. } & (x, y) \in \text{ellipsoid} \\ & x \in \{0, 1, 2, 3\} \\ & y \in [0, 3] \end{aligned}$$



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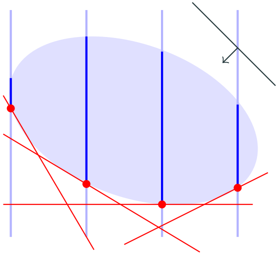

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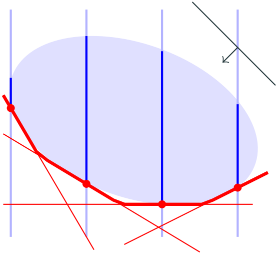

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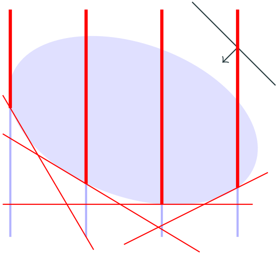

Outer Approximation Method (OA), ECP, EHP

Convex MINLP

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Outer Approximation (OA) algorithm

[Duran and Grossmann, 1986]:

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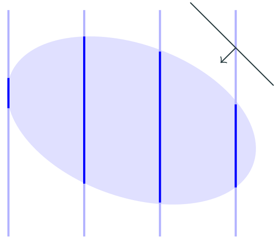

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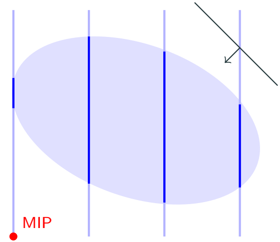

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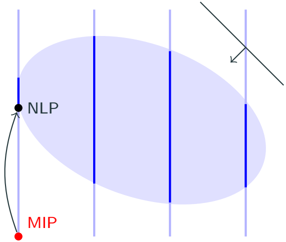

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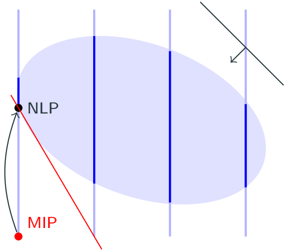

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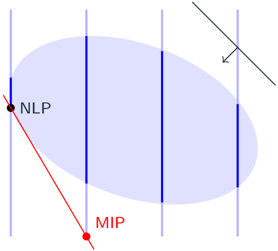

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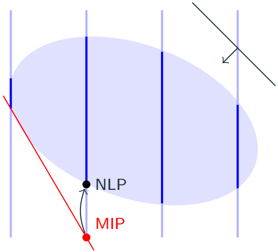

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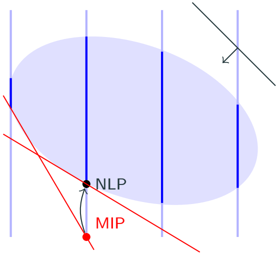

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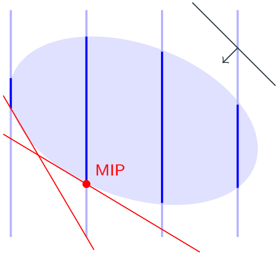
Outer Approximation (OA) algorithm

[Duran and Grossmann, 1986]:

- Start with $R := \emptyset$.
- Dynamically increase R by alternatively solving MIP relaxations and NLP subproblems until MIP solution is feasible for MINLP.



Outer Approximation Method (OA), ECP, EHP

Convex MINLP

$$\begin{aligned} \min\ & c^{\mathsf T} x \\ \text{s.t. } & g_k(x) \le 0 && \forall k \in [m] \\ & x_i \in \mathbb{Z} && \forall i \in \mathcal{I} \subseteq [n] \\ & x_i \in [\ell_i, u_i] && \forall i \in [n] \end{aligned}$$

$$\equiv$$

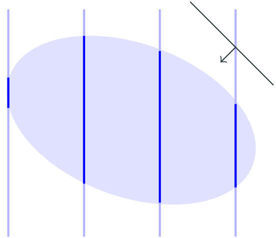
MIP

$$\begin{aligned} \min\ & c^{\mathsf T} x, \\ \text{s.t. } & g_k(\hat{x}) + \nabla g_k(\hat{x})^{\mathsf T}(x - \hat{x}) \le 0, \\ & \qquad \forall k \in [m], \quad \hat{x} \in R, \\ & x_i \in \mathbb{Z}, \quad \forall i \in \mathcal{I}, \\ & x_i \in [\ell_i, u_i], \quad \forall i \in [n] \end{aligned}$$

Extended Cutting Plane Method (ECP)

[Kelley, 1960, Westerlund and Petterson, 1995]:

- Iteratively solve MIP relaxation only.
- Linearize $g_k(\cdot)$ in MIP relaxation.
- No need to solve NLP, but weaker MIP relaxation.



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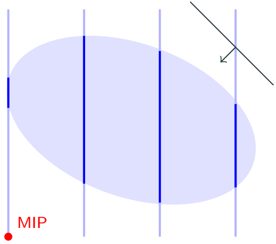

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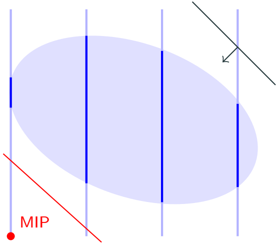

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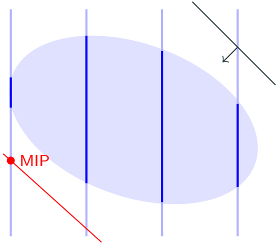

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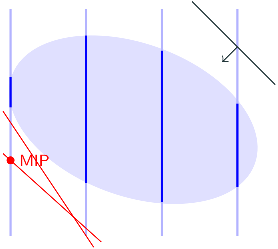

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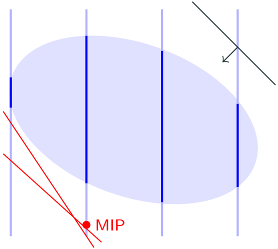

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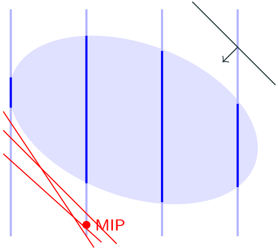

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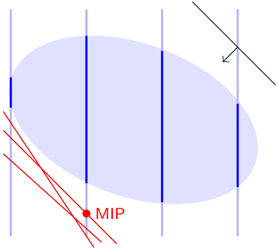

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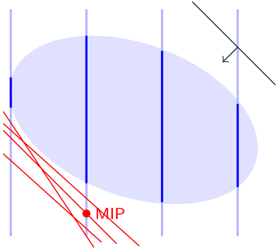

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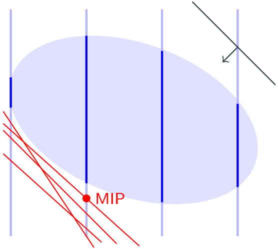

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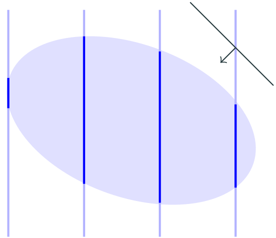

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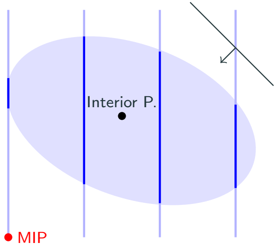

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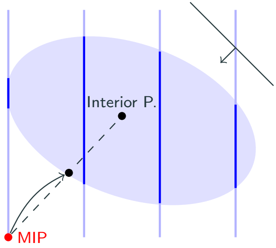

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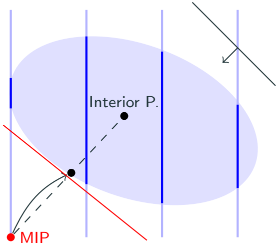

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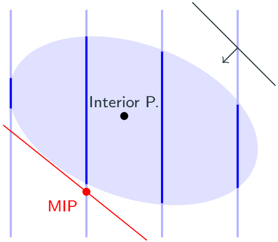

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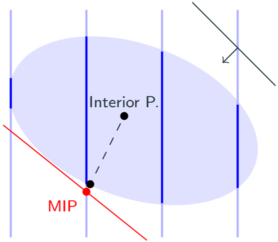

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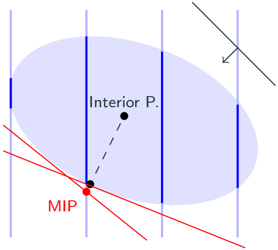


Convex MINLP

$$\begin{aligned} \min\ & c^{\mathsf{T}} x \\ \text{s.t. } & g_k(x) \le 0 && \forall k \in [m] \\ & x_i \in \mathbb{Z} && \forall i \in \mathcal{I} \subseteq [n] \\ & x_i \in [\ell_i, u_i] && \forall i \in [n] \end{aligned}$$

$\equiv$

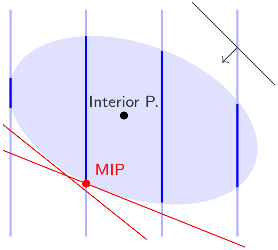
MIP

$$\begin{aligned} \min\ & c^{\mathsf{T}} x, \\ \text{s.t. } & g_k(\hat{x}) + \nabla g_k(\hat{x})^{\mathsf{T}} (x - \hat{x}) \le 0, \\ & \qquad \forall k \in [m], \quad \hat{x} \in R, \\ & x_i \in \mathbb{Z}, \quad \forall i \in \mathcal{I}, \\ & x_i \in [\ell_i, u_i], \quad \forall i \in [n] \end{aligned}$$

Extended Hyperplane Method (EHP)

[Veinott, 1967, Kronqvist, Lundell, and Westerlund, 2016]:

- Iteratively solve MIP relaxation only.
- Move MIP solution onto NLP-feasible set $\{x \in [\ell, u] : g_k(x) \le 0\}$ via linesearch.
- Linearize $g_k(\cdot)$ in improved reference point.
- No need to solve NLP, but stronger MIP than ECP.



LP/NLP- or LP-based Branch & Bound

OA/ECP/EHP: Solving a sequence of MIP relaxations can be expensive and wasteful (no warmstarts)

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- Integrate NLP-solves into MIP Branch & Bound.
- When LP relaxation is integer feasible, solve NLP subproblem (as in OA).
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LP-based Branch & Bound:

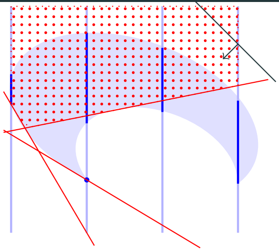
- Integrate Kelley' Cutting Plane method into MIP Branch & Bound.
- Add linearization in LP solution to LP relaxation (as in ECP).
- Optional: Move LP solution onto NLP-feasible set $\{x \in [\ell, u] : g_k(x) \leq 0\}$ via linesearch (as in EHP) [Maher, Fischer, Gally, Gamrath, Gleixner, Gottwald, Hendel, Koch, Lübbecke, Miltenberger, Müller, Pfetsch, Puchert, Rehfeldt, Schenker, Schwarz, Serrano, Shinano, Weninger, Witt, and Witzig, 2017].

Fundamental Methods

Nonconvex MINLP

Nonconvex MINLP

Now: Let $g_k(\cdot)$ be nonconvex for some $k \in [m]$.



Outer-Approximation:

- Linearizations
  $g_k(\hat{x}) + \nabla g_k(\hat{x})(x - \hat{x}) \leq 0$
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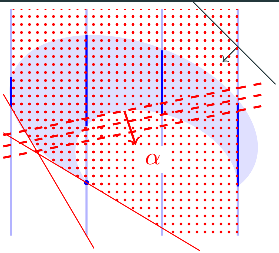
NLP-based Branch & Bound:

- Solving nonconvex NLP relaxation to global optimality can be as hard as original problem.



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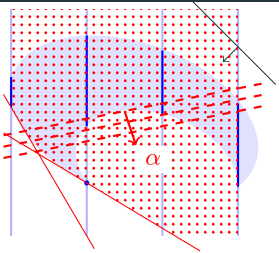

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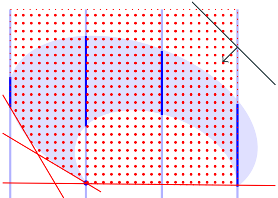

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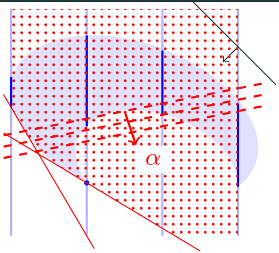

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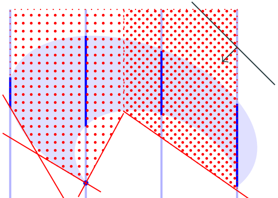

Convex Relaxation

Given: $X = \{x \in [\ell, u] \,:\, g_k(x) \leq 0, k \in [m]\}$ (continuous relaxation of MINLP)

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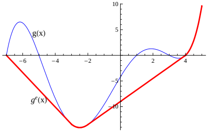
$$\{x \in [\ell, u] \, : \, \text{“}\mathrm{conv}(g_k)\text{''}(x) \leq 0\}$$



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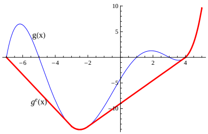

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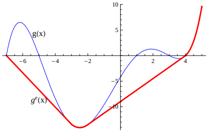

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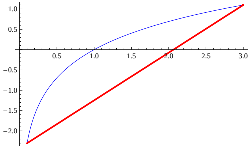
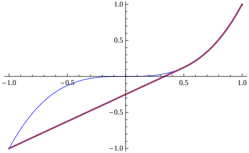
- In practice, convex envelope is not known explicitly in general
  – **except for many “simple functions”**

Convex Envelopes for “simple” functions

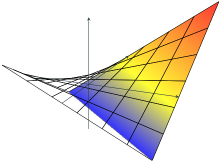
concave functions



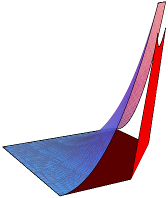
$x^k \quad (k \in 2\mathbb{Z}+1)$



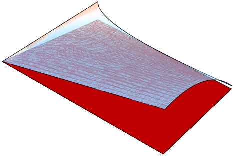
$x \cdot y$



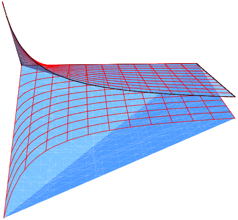
$x^2 \cdot y^2$



$-\sqrt{x} \cdot y^2$



$x/y \quad (0 < y < \infty)$



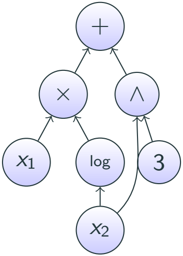
Factorable Functions [McCormick, 1976]

$g(x)$ is factorable if it can be expressed as a combination of functions from a finite set of operators, e.g., $\{+, \times, \div, \wedge, \sin, \cos, \exp, \log, |\cdot|\}$, whose arguments are variables, constants, or other factorable functions.

- Typically represented as expression trees or graphs (DAG).
- Excludes integrals $x \mapsto \int_{x_0}^{x} h(\zeta) d\zeta$ and black-box functions.

Example:

$$x_1 \log(x_2) + x_2^3$$



Reformulation of Factorable MINLP

Smith and Pantelides [1996, 1997]: By introducing new variables and equations, every factorable MINLP can be **reformulated** such that for every constraint function the convex envelope is known.

$$
\begin{array}{l}
x_1 \log(x_2) + x_2^3 \le 0 \\
x_1 \in [1,2],\ x_2 \in [1,e]
\end{array}
\quad \overset{}{\underset{\text{Reform}}{\Longrightarrow}} \quad
\begin{array}{l}
y_1 + y_2 \le 0 \\
x_1 y_3 = y_1 \\
x_2^3 = y_2 \\
\log(x_2) = y_3 \\
x_1 \in [1,2],\ x_2 \in [1,e] \\
y_1 \in [0,2],\ y_2 \in [1,e^3] \\
y_3 \in [0,1]
\end{array}
$$

- Bounds for new variables inherited from functions and their arguments, e.g., $y_3 \in \log([1,e]) = [0,1]$.
- Reformulation may not be unique, e.g., $xyz = (xy)z = x(yz)$.

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$$x_1 \log(x_2) + x_2^3 \le 0$$
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$\Longrightarrow$ Reform

$$\begin{aligned} y_1 + y_2 &\le 0 \\ x_1 y_3 &= y_1 \\ x_2^3 &= y_2 \\ \log(x_2) &= y_3 \end{aligned}$$
$$x_1 \in [1,2],\ x_2 \in [1,e]$$
$$y_1 \in [0,2],\ y_2 \in [1,e^3]$$
$$y_3 \in [0,1]$$

$\Longrightarrow$ Convex Relax

$$\begin{aligned} y_1 + y_2 &\le 0 \\ 2y_3 + x_1 - 2 &\le y_1 \\ y_3 &\le y_1 \\ y_1 &\le 2y_3 \\ y_1 &\le y_3 + x - 1 \\ x_2^3 &\le y_2 \\ y_2 &\le 1 + \frac{e^3-1}{e-1}(x_2 - 1) \\ \frac{1}{e-1}(x_2 - 1) &\le y_3 \\ y_3 &\le \log(x_2) \end{aligned}$$
$$x_1 \in [1,2],\ x_2 \in [1,e]$$
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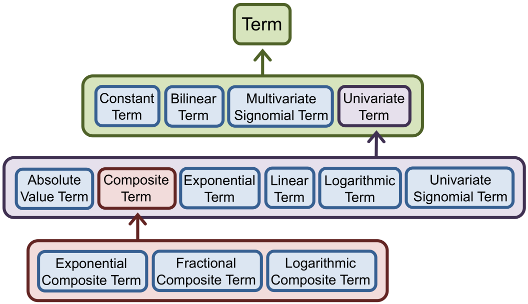
Factorable Reformulation in Practice

The type of algebraic expressions that is understood and not broken up further is implementation specific.

Thus, not all functions are supported by any deterministic solver, e.g.,

- ANTIGONE, BARON, and SCIP do not support trigonometric functions.
- Couenne does not support max or min.
- No deterministic global solver supports external functions that are given by routines for point-wise evaluation of function and derivatives.

Example ANTIGONE [Misener and Floudas, 2014]:



Spatial Branching

Recall **Spatial Branch & Bound**:

- ✓ **Relax nonconvexity** to obtain a tractable relaxation (often an LP).
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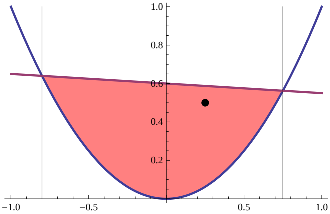
The variable bounds determine the convex relaxation, e.g., for the constraint

$$y = x^2, \qquad x \in [\ell, u],$$

the convex relaxation is

$$x^2 \leq y \leq \ell^2 + \frac{u^2 - \ell^2}{u - \ell}(x - \ell), \qquad x \in [\ell, u].$$



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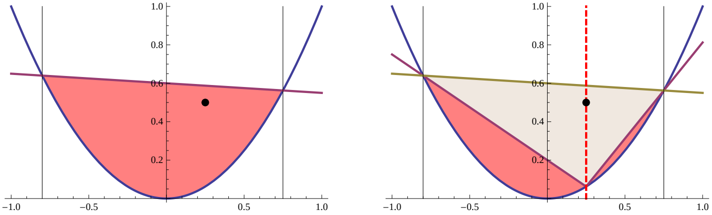
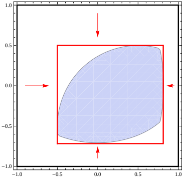
Thus, branching on a nonlinear variable in a nonconvex term allows for tighter relaxations in sub-problems:



Fundamental Methods

Bound Tightening

Variable Bounds Tightening (Domain Propagation)



Tighten variable bounds $[\ell, u]$ 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.

Formally:

$$\min / \max \{x_k \; : \; x \in \mathcal{R}\}, \qquad k \in [n],$$

where $\mathcal{R} = \{x \in [\ell, u] : g(x) \leq 0, x_i \in \mathbb{Z}, i \in \mathcal{I}\}$ (MINLP-feasible set) or a relaxation thereof.

Bound tightening can **tighten the LP relaxation without branching**.

Belotti, Lee, Liberti, Margot, and Wächter [2009]: overview on bound tightening for MINLP

Feasbility-based Bound Tightening (FBBT):

Deduce variable bounds from single constraint and box $[\ell, u]$, that is

$$\mathcal{R} = \{x \in [\ell, u] \ : \ g_j(x) \leq 0\} \qquad \text{for some fixed } j \in [m].$$

- cheap and effective ⇒ used for "probing"

Feasibility-Based Bound Tightening

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- cheap and effective $\Rightarrow$ used for "probing"

Linear Constraints:

$$b \leq \sum_{i:a_i>0} a_i x_i + \sum_{i:a_i<0} a_i x_i \leq c, \qquad \ell \leq x \leq u$$

$$\Rightarrow \qquad x_j \leq \frac{1}{a_j} \begin{cases} c - \sum\limits_{i:a_i>0, i\neq j} a_i \ell_i - \sum\limits_{i:a_i<0} a_i u_i, & \text{if } a_j > 0 \\ b - \sum\limits_{i:a_i>0} a_i u_i - \sum\limits_{i:a_i<0, i\neq j} a_i \ell_i, & \text{if } a_j < 0 \end{cases}$$

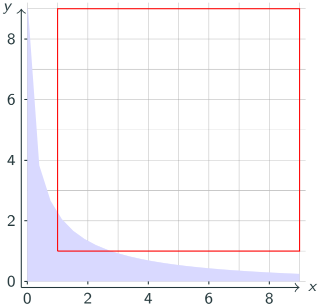
$$x_j \geq \frac{1}{a_j} \begin{cases} b - \sum\limits_{i:a_i>0, i\neq j} a_i u_i - \sum\limits_{i:a_i<0} a_i \ell_i, & \text{if } a_j > 0 \\ c - \sum\limits_{i:a_i>0} a_i \ell_i - \sum\limits_{i:a_i<0, i\neq j} a_i u_i, & \text{if } a_j < 0 \end{cases}$$

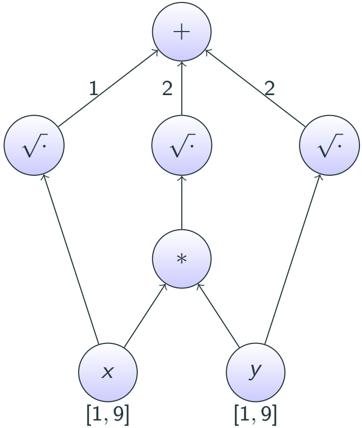
- Belotti, Cafieri, Lee, and Liberti [2010]: fixed point of iterating FBBT on set of linear constraints can be computed by solving one LP
- Belotti [2013]: FBBT on **two** linear constraints simultaneously

Example:

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

$$x, y \in [1, 9]$$





Feasibility-Based Bound Tightening on Expression “Tree”

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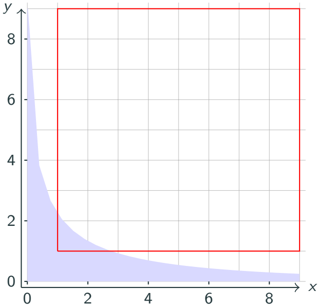
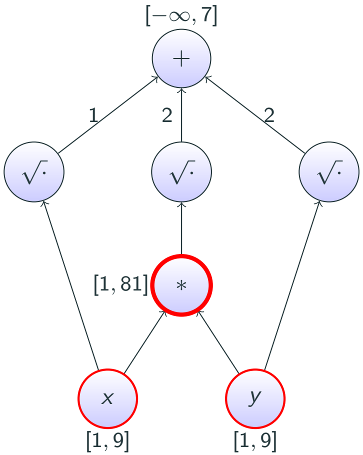


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)



$[1, 9] * [1, 9] = [1, 81]$

Application of **Interval Arithmetics**

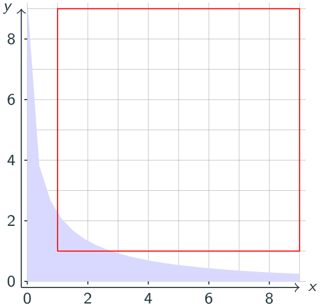
[Moore, 1966]

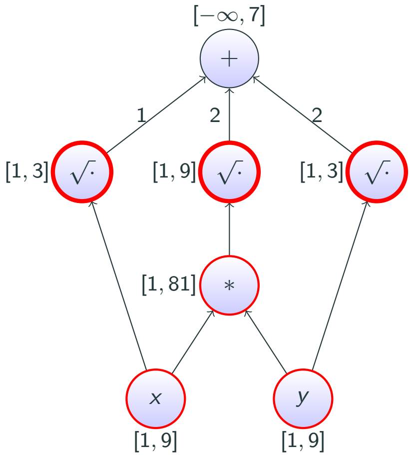
Feasibility-Based Bound Tightening on Expression "Tree"

Example:

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

$$x, y \in [1, 9]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

$\sqrt{[1,9]} = [1,3] \qquad \sqrt{[1,81]} = [1,9]$

Application of **Interval Arithmetics**

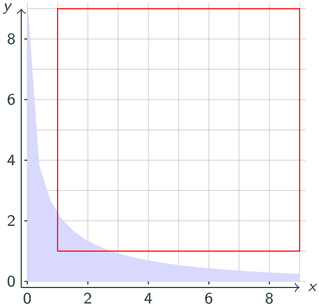
[Moore, 1966]

Feasibility-Based Bound Tightening on Expression "Tree"

Example:

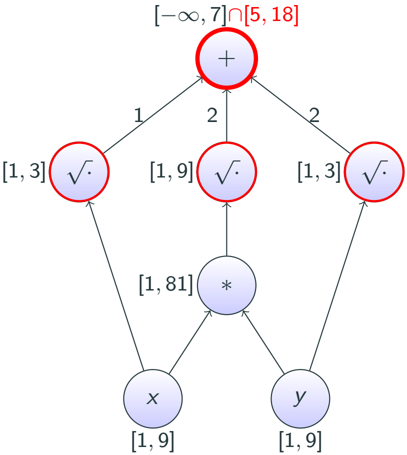
$$\sqrt{x} + 2\sqrt{xy} + 2\sqrt{y} \in [-\infty, 7]$$

$$x, y \in [1, 9]$$



Forward propagation:

- compute bounds on intermediate nodes (bottom-up)



$$[1, 3] + 2\,[1, 9] + 2\,[1, 3] = [5, 18]$$

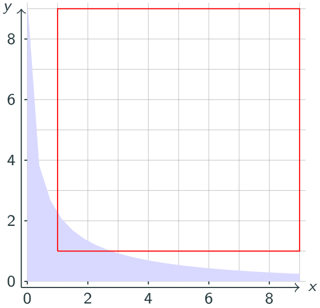
Application of **Interval Arithmetics**

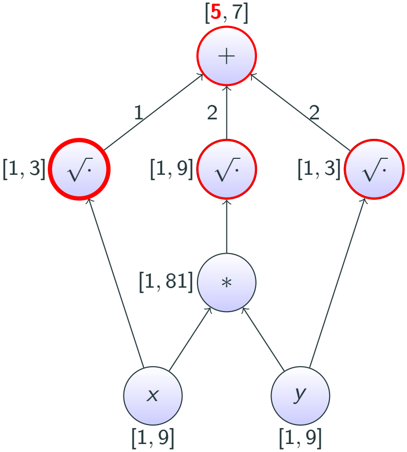
[Moore, 1966]

Example:

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

$$x, y \in [1, 9]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

$$[5, 7] - 2\,[1, 9] - 2\,[1, 3] = [-19, 3]$$

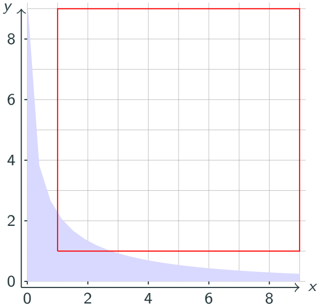
Application of **Interval Arithmetics**

[Moore, 1966]

Example:

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

$$x, y \in [1, 9]$$

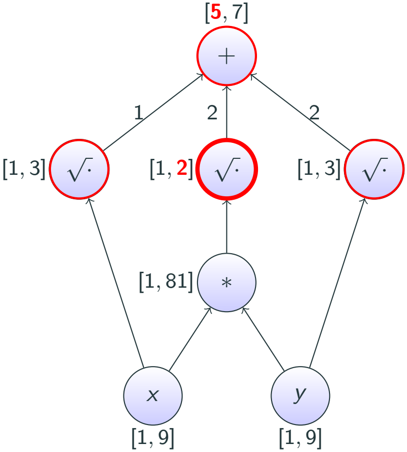


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$$([5, 7] - [1, 3] - 2\,[1, 3])/2 = [-2, 2]$$

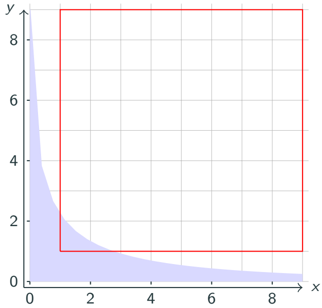
Application of **Interval Arithmetics**

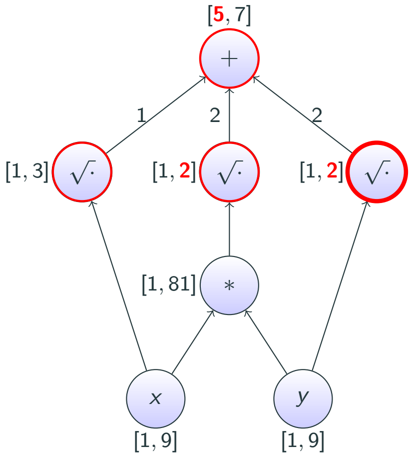
[Moore, 1966]

Example:

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

$$x, y \in [1, 9]$$





$$([5,7] - [1,3] - 2\,[1,2])/2 = [-1,2]$$

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

Application of **Interval Arithmetics**

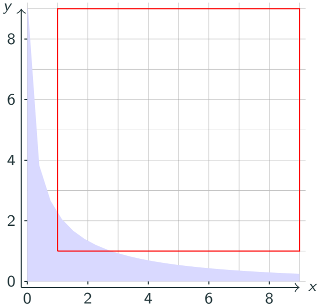
[Moore, 1966]

Feasibility-Based Bound Tightening on Expression "Tree"

Example:

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

$$x, y \in [1, 9]$$

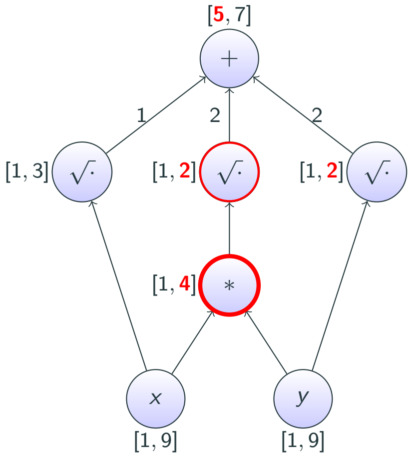


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$[1, 2]^2 = [1, 4]$

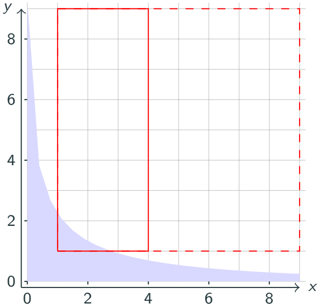
Application of **Interval Arithmetics**

[Moore, 1966]

Example:

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

$$x, y \in [1, 9]$$

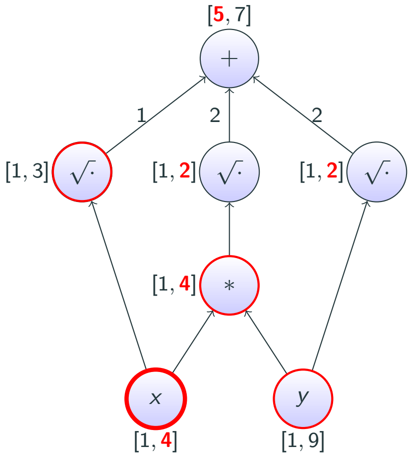


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$[1, 3]^2 = [1, 9]$ $\quad$ $[1, 4]/[1, 9] = [1/9, 4]$

Application of **Interval Arithmetics**

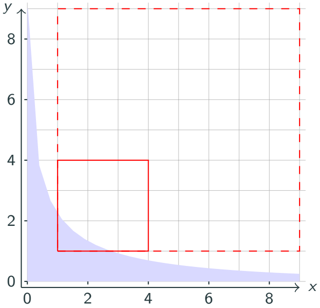
[Moore, 1966]

Feasibility-Based Bound Tightening on Expression “Tree”

Example:

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

$$x, y \in [1, 9]$$

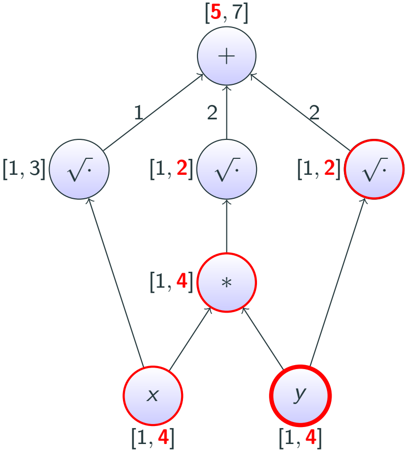


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$[1, 2]^2 = [1, 4] \qquad [1, 4]/[1, 4] = [1/4, 4]$

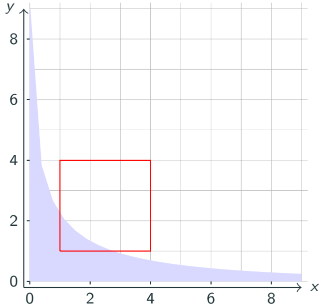
Application of **Interval Arithmetics**

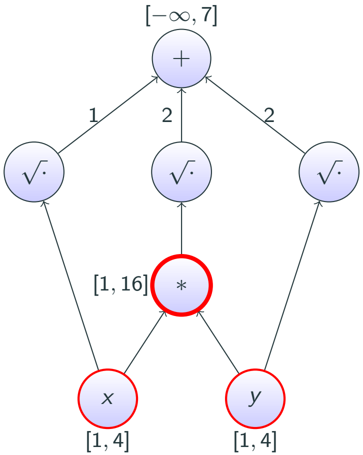
[Moore, 1966]

Example:

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

$$x, y \in [1, 4]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

$[1, 4] * [1, 4] = [1, 16]$

Backward propagation:

- reduce bounds using reverse operations (top-down)

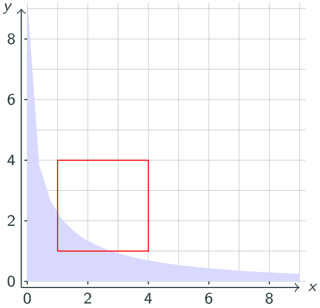
Application of **Interval Arithmetics**

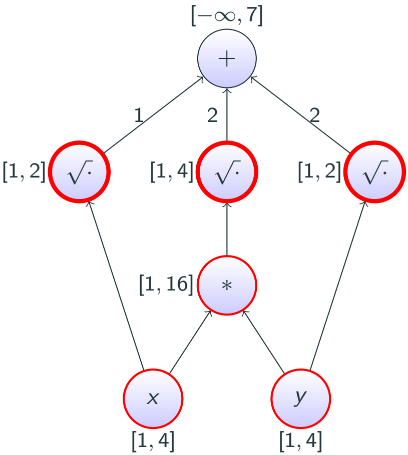
[Moore, 1966]

Example:

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

$$x, y \in [1, 4]$$





$\sqrt{[1,4]} = [1,2]$ $\quad$ $\sqrt{[1,16]} = [1,4]$

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

Application of **Interval Arithmetics**

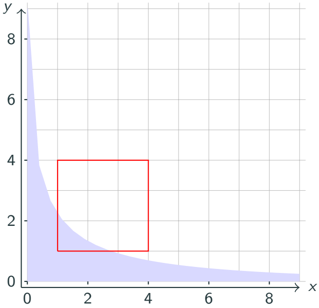
[Moore, 1966]

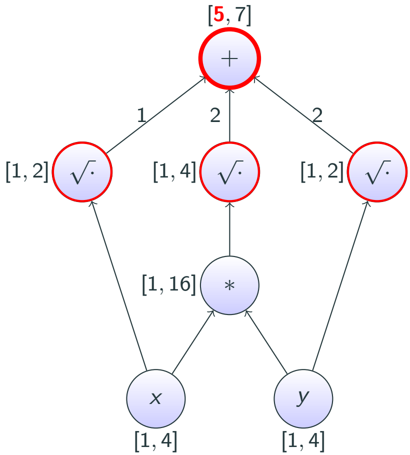
Feasibility-Based Bound Tightening on Expression "Tree"

Example:

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

$$x, y \in [1, 4]$$





$$[1, 2] + 2\,[1, 4] + 2\,[1, 2] = [5, 14]$$

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

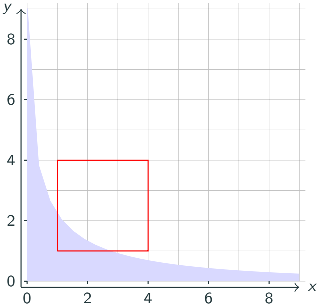
Application of **Interval Arithmetics**

[Moore, 1966]

Example:

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

$$x, y \in [1, 4]$$

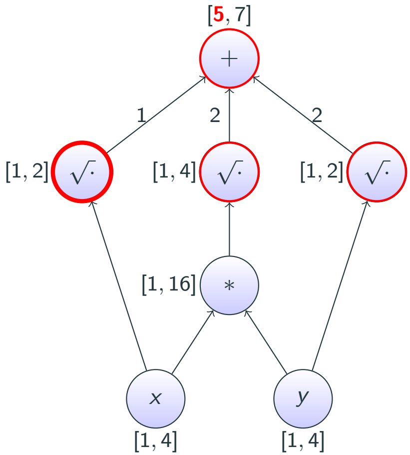


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$$[5, 7] - 2\,[1, 4] - 2\,[1, 2] = [-7, 3]$$

Application of **Interval Arithmetics**

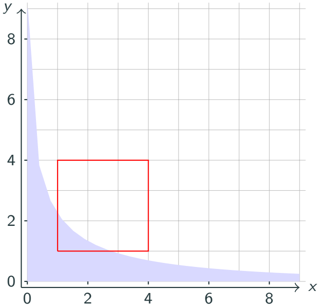
[Moore, 1966]

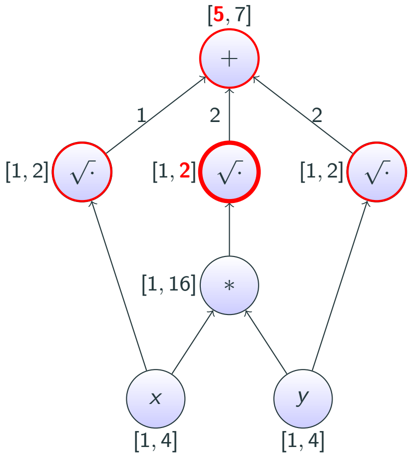
Feasibility-Based Bound Tightening on Expression "Tree"

Example:

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

$$x, y \in [1, 4]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

$$([5, 7] - [1, 2] - 2\,[1, 2])/2 = [-0.5, 2]$$

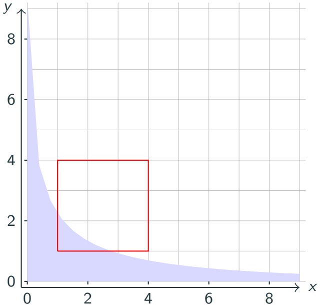
Application of **Interval Arithmetics**

[Moore, 1966]

Example:

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

$$x, y \in [1, 4]$$

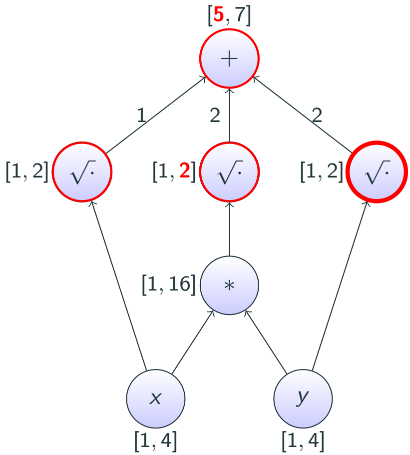


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



$$([5, 7] - [1, 2] - 2\,[1, 4])/2 = [-2.5, 2]$$

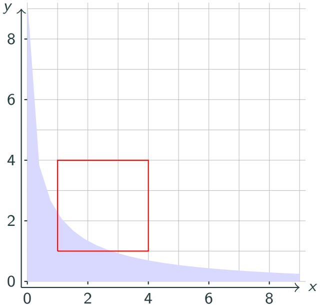
Application of **Interval Arithmetics**

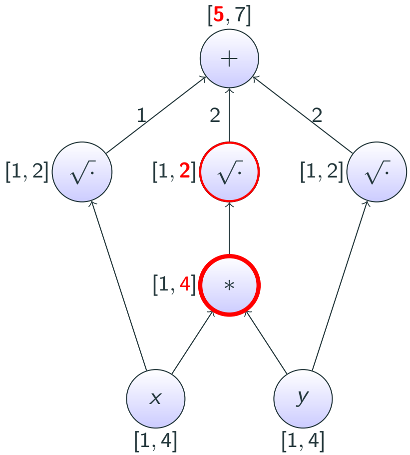
[Moore, 1966]

Example:

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

$$x, y \in [1, 4]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

$[1, 2]^2 = [1, 4]$

Application of **Interval Arithmetics**

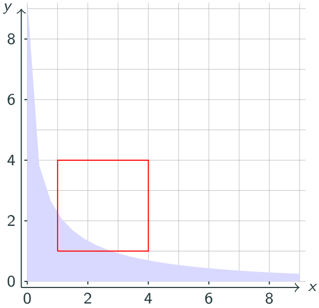
[Moore, 1966]

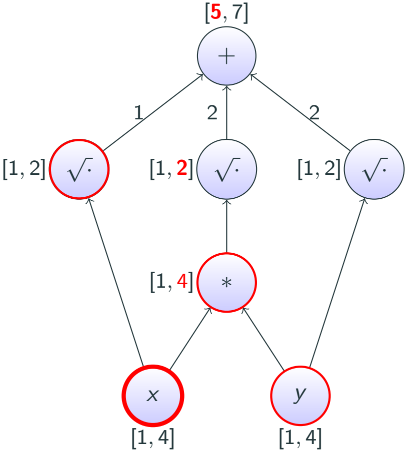
Feasibility-Based Bound Tightening on Expression "Tree"

Example:

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

$$x, y \in [1, 4]$$





Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

$[1, 2]^2 = [1, 4]$ $\quad$ $[1, 4]/[1, 4] = [1/4, 4]$

Application of **Interval Arithmetics**

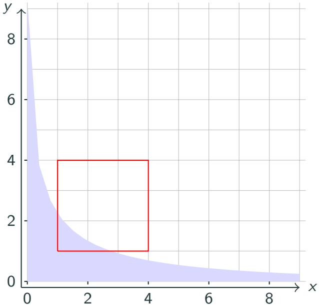
[Moore, 1966]

Feasibility-Based Bound Tightening on Expression “Tree”

Example:

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

$$x, y \in [1, 4]$$



Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

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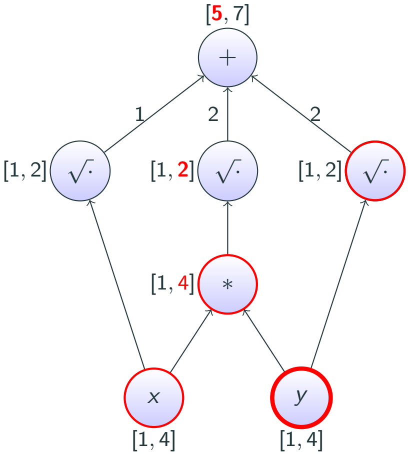


$[1, 2]^2 = [1, 4]$ $\quad$ $[1, 4]/[1, 4] = [1/4, 4]$

Application of **Interval Arithmetics**

[Moore, 1966]

Problem: Overestimation

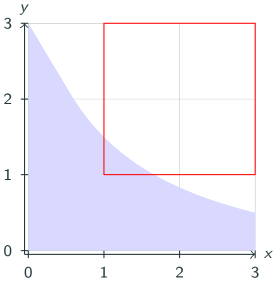
FBBT with Bivariate Quadratics

Example – reformulated:

$(x' = \sqrt{x},\ y' = \sqrt{y})$

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$

$$x', y' \in [1, 3]$$



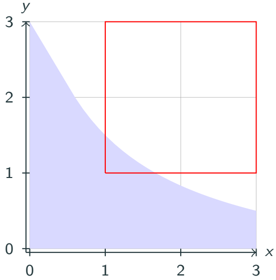
Simple FBBT:

$$x' \leq 7 - 2x'y' - 2y'$$

$$x' \leq (7 - x' - 2y')/(2y')$$

Example – reformulated:
($x' = \sqrt{x}$, $y' = \sqrt{y}$)

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$
$$x', y' \in [1, 3]$$



Simple FBBT:

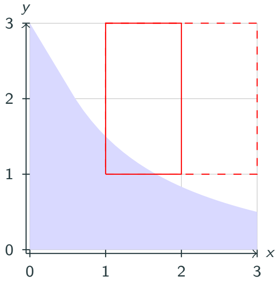
$$\begin{aligned} x' &\leq 7 - 2x'y' - 2y' \\ &\leq 7 - 2 \cdot 1 \cdot 1 - 2 \cdot 1 \\ x' &\leq (7 - x' - 2y')/(2y') \\ &\leq (7 - 1 - 2 \cdot 1)/(2 \cdot 1) \end{aligned}$$

Example – reformulated:

$(x' = \sqrt{x},\ y' = \sqrt{y})$

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$

$$x', y' \in [1, 3]$$



Simple FBBT:

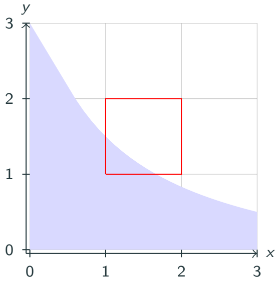
$$\begin{aligned} x' &\le 7 - 2x'y' - 2y' \\ &\le 7 - 2\cdot 1 \cdot 1 - 2 \cdot 1 = \mathbf{3} \\ x' &\le (7 - x' - 2y')/(2y') \\ &\le (7 - 1 - 2\cdot 1)/(2\cdot 1) = \mathbf{2} \end{aligned}$$

FBBT with Bivariate Quadratics

Example – reformulated:

$(x' = \sqrt{x},\ y' = \sqrt{y})$

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$
$$x', y' \in [1, 3]$$

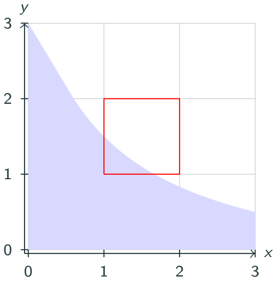


Simple FBBT:

$$\begin{aligned} x' &\le 7 - 2x'y' - 2y' \\ &\le 7 - 2\cdot 1\cdot 1 - 2\cdot 1 = \mathbf{3} \\ x' &\le (7 - x' - 2y')/(2y') \\ &\le (7 - 1 - 2\cdot 1)/(2\cdot 1) = \mathbf{2} \\ y' &\le (7 - 2x'y' - x')/2 \le \mathbf{2} \\ y' &\le (7 - 2y' - x')/(2x') \le \mathbf{2} \end{aligned}$$

Example – reformulated:
($x' = \sqrt{x}$, $y' = \sqrt{y}$)

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$
$$x', y' \in [1, 3]$$



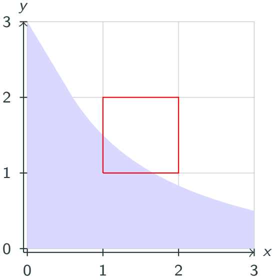
Simple FBBT:

$$\begin{aligned} x' &\leq 7 - 2x'y' - 2y' \\ &\leq 7 - 2 \cdot 1 \cdot 1 - 2 \cdot 1 = \mathbf{3} \\ x' &\leq (7 - x' - 2y')/(2y') \\ &\leq (7 - 1 - 2 \cdot 1)/(2 \cdot 1) = \mathbf{2} \\ y' &\leq (7 - 2x'y' - x')/2 \leq \mathbf{2} \\ y' &\leq (7 - 2y' - x')/(2x') \leq \mathbf{2} \end{aligned}$$

FBBT with Bivariate Quadratics

Example – reformulated:
($x' = \sqrt{x}$, $y' = \sqrt{y}$)

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$
$$x', y' \in [1, 3]$$



Simple FBBT:

$$\begin{aligned} x' &\leq 7 - 2x'y' - 2y' \\ &\leq 7 - 2 \cdot 1 \cdot 1 - 2 \cdot 1 = \mathbf{3} \\ x' &\leq (7 - x' - 2y')/(2y') \\ &\leq (7 - 1 - 2 \cdot 1)/(2 \cdot 1) = \mathbf{2} \\ y' &\leq (7 - 2x'y' - x')/2 \leq \mathbf{2} \\ y' &\leq (7 - 2y' - x')/(2x') \leq \mathbf{2} \end{aligned}$$

Consider Bivariate Quadratic as **one term**
[Vigerske, 2013, Vigerske and Gleixner, 2017]:

$$x' \leq \frac{7 - 2y'}{1 + 2y'}$$
$$y' \leq \frac{7 - x'}{2 + 2x'}$$

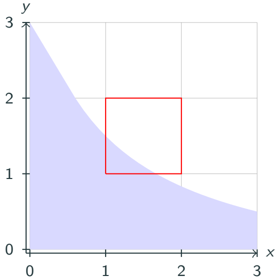
FBBT with Bivariate Quadratics

Example – reformulated:

$(x' = \sqrt{x},\ y' = \sqrt{y})$

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$

$$x', y' \in [1, 3]$$

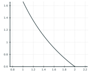


Simple FBBT:

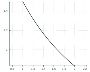
$$\begin{aligned} x' &\le 7 - 2x'y' - 2y' \\ &\le 7 - 2 \cdot 1 \cdot 1 - 2 \cdot 1 = \mathbf{3} \\ x' &\le (7 - x' - 2y')/(2y') \\ &\le (7 - 1 - 2 \cdot 1)/(2 \cdot 1) = \mathbf{2} \\ y' &\le (7 - 2x'y' - x')/2 \le \mathbf{2} \\ y' &\le (7 - 2y' - x')/(2x') \le \mathbf{2} \end{aligned}$$

Consider Bivariate Quadratic as **one term** [Vigerske, 2013, Vigerske and Gleixner, 2017]:

$$x' \le \frac{7 - 2y'}{1 + 2y'}$$



$$y' \le \frac{7 - x'}{2 + 2x'}$$



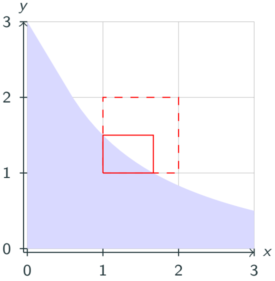
FBBT with Bivariate Quadratics

Example – reformulated:

$(x' = \sqrt{x},\ y' = \sqrt{y})$

$$x' + 2x'y' + 2y' \in [-\infty, 7]$$

$$x', y' \in [1, 3]$$



Simple FBBT:

$$\begin{aligned} x' &\le 7 - 2x'y' - 2y' \\ &\le 7 - 2\cdot 1 \cdot 1 - 2 \cdot 1 = \mathbf{3} \\ x' &\le (7 - x' - 2y')/(2y') \\ &\le (7 - 1 - 2\cdot 1)/(2 \cdot 1) = \mathbf{2} \\ y' &\le (7 - 2x'y' - x')/2 \le \mathbf{2} \\ y' &\le (7 - 2y' - x')/(2x') \le \mathbf{2} \end{aligned}$$

Consider Bivariate Quadratic as **one term**

[Vigerske, 2013, Vigerske and Gleixner, 2017]:

$$x' \le \frac{7 - 2y'}{1 + 2y'} \le \frac{7 - 2\cdot 1}{1 + 2 \cdot 1} = \mathbf{\frac{5}{3}}$$

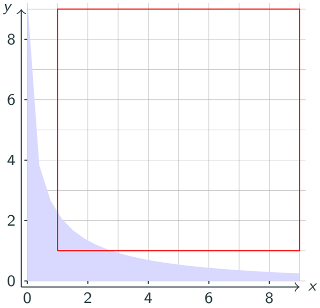
$$y' \le \frac{7 - x'}{2 + 2x'} \le \frac{7 - 1}{2 + 2 \cdot 1} = \mathbf{\frac{3}{2}}$$

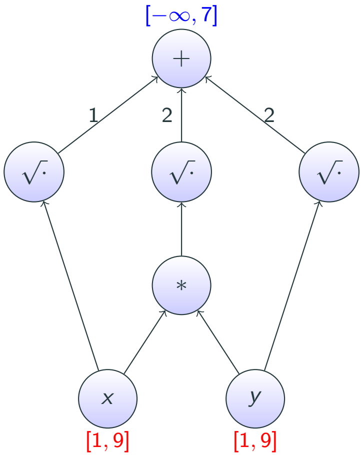
FBBT on Expression Graph

Example:

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

$x, y \in [1, 9]$





- Common subexpressions from different constraints may stronger boundtightening.

FBBT on Expression Graph

Example:

$$\sqrt{x} + 2\sqrt{xy} + 2\sqrt{y} \in [-\infty, 7]$$
$$x^2\sqrt{y} - 2xy + 3\sqrt{y} \in [0, 2]$$
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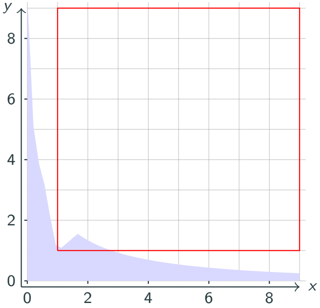

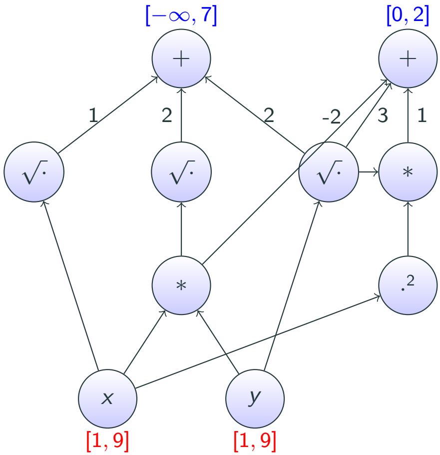

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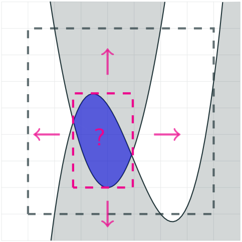
Acceleration – Selected Topics

Acceleration – Selected Topics

Optimization-based bound tightening

Optimization-based bound tightening

Recall: Bound Tightening $\equiv \min / \max \{x_k \, : \, x \in \mathcal{R}\}$, $k \in [n]$, where
$\mathcal{R} \supseteq \{x \in [\ell, u] : g(x) \leq 0, x_i \in \mathbb{Z}, i \in \mathcal{I}\}$



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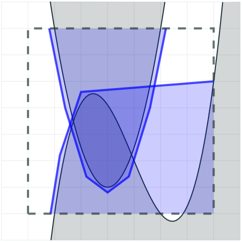
Optimization-based Bound Tightening

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

- $\mathcal{R} = \{x : Ax \leq b, c^\top x \leq z^*\}$ linear relaxation (with obj. cutoff)



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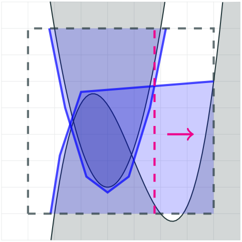

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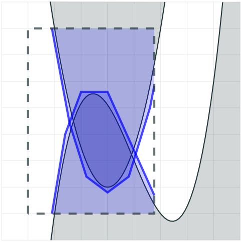
- but: potentially many expensive LPs per node



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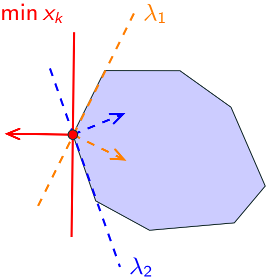


Advanced implementation [Gleixner, Berthold, Müller, and Weltge, 2017]:

- solve OBBT LPs at root only, learn dual certificates $x_k \geq \sum_i r_i x_i + \mu z^* + \lambda^{\mathsf{T}} b$
- propagate duality certificates during tree search ("approximate OBBT")
- greedy ordering for faster LP warmstarts, filtering of provably tight bounds
- 16% faster (24% on instances $\geq$ 100 seconds) and less time outs

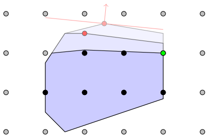
Acceleration – Selected Topics

Synergies with MIP and NLP

MIP ⊂ MINLP

Many MIP techniques can be generalized for MINLP

- MIP cutting planes applied to LP relaxation, e.g., Gomory, Mixed-Integer Rounding, Flow Cover
- MIP cutting planes generalized to MINLP, e.g., Disjunctive Cuts [Kilinç, Linderoth, and Luedtke, 2010, Belotti, 2012, Bonami, Linderoth, and Lodi, 2012]



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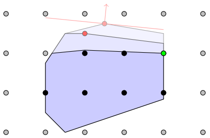

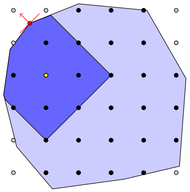

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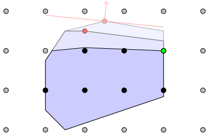
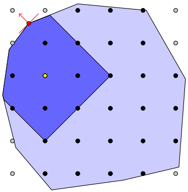
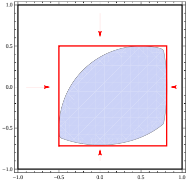
- Bound Tightening







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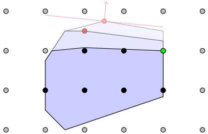
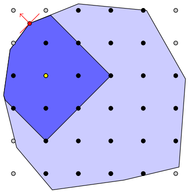
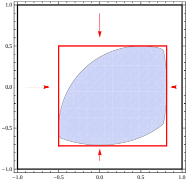
- Bound Tightening
- Symmetry detection and breaking [Liberti, 2012, Liberti and Ostrowski, 2014]



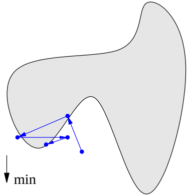




NLP ⊂ MINLP

NLP Solvers (finding local optima) are used in MINLP solver

- to find feasible points when integrality and linear constraints are satisfied
- to solve continuous relaxation in NLP-based B&B



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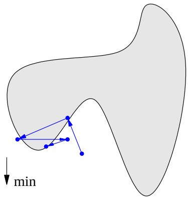
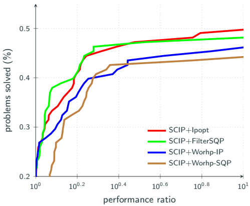
- performance of NLP solver is problem-dependent
- some MINLP solvers interface several NLP solvers:

  ANTIGONE: CONOPT, SNOPT

  BARON: FilterSD, FilterSQP, GAMS/NLP (e.g., CONOPT), IPOPT, MINOS, SNOPT

  SCIP (next ver.): FilterSQP, IPOPT, WORHP





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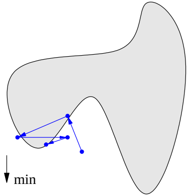
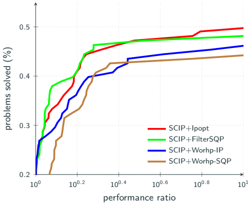
  BARON: FilterSD, FilterSQP, GAMS/NLP (e.g., CONOPT), IPOPT, MINOS, SNOPT
  SCIP (next ver.): FilterSQP, IPOPT, WORHP
- strategy to select NLP solver becomes important: e.g., in SCIP, always choosing best NLP solver finds 10% more locally optimal points and is 2–3x faster than best single solver [Müller et al., 2017]
- BARON chooses according to solver performance
- "fast fail" on expensive NLPs, warmstart in B&B seem important [Müller et al., 2017, Mahajan et al., 2012]





Acceleration – Selected Topics

Convexity

Convexity Detection

Analyze the Hessian:

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

- $f(x)$ quadratic: $\nabla^2 f(x)$ constant $\Rightarrow$ compute spectrum numerically
- general $f \in C^2$: estimate eigenvalues of Interval-Hessian [Nenov et al., 2004]

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Analyze the Algebraic Expression:

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

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

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

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

[Maranas and Floudas, 1995, Bao, 2007, Fourer, Maheshwari, Neumaier, Orban, and Schichl, 2009, Vigerske, 2013]

Second Order Cones (SOC)

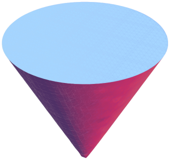
Consider a constraint $\quad x^{\mathsf{T}}Ax + b^{\mathsf{T}}x \leq c.$

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

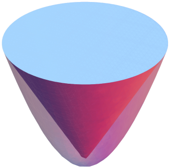
$$\sum_{k=1}^{N} x_k^2 - x_{N+1}^2 \leq 0, x_{N+1} \geq 0 \qquad \Leftrightarrow \qquad \sqrt{\sum_{k=1}^{N} x_k^2} \leq x_{N+1}$$

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

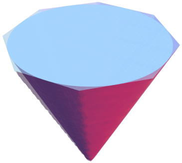
Example: $x^2 + y^2 - z^2 \leq 0$ in $[-1,1] \times [-1,1] \times [0,1]$



feasible region



not recognizing SOC



recognizing SOC

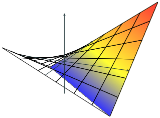
(initial relaxation)

Acceleration – Selected Topics

Convexification

Bilinear $x \cdot y$ $\quad (x \in [\ell_x, u_x],\ y \in [\ell_y, u_y])$:

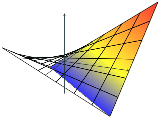
$$\max \left\{ \begin{array}{c} u_x y + u_y x - u_x u_y \\ \ell_x y + \ell_y x - \ell_x \ell_y \end{array} \right\} \leq x \cdot y \leq \min \left\{ \begin{array}{c} u_x y + \ell_y x - u_x \ell_y \\ \ell_x y + u_y x - \ell_x u_y \end{array} \right\}$$



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

Convex Envelopes for Product Terms

Bilinear $x \cdot y$ $\quad (x \in [\ell_x, u_x],\ y \in [\ell_y, u_y])$:



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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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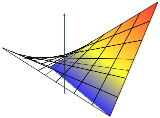

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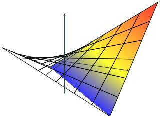
- if mixed signs (e.g., $\ell_x < 0 < u_x$) recursion may not provide convex envelope
- Meyer and Floudas [2004] derive the facets of the envelopes: for convex envelope, distinguish 9 cases, each giving 5-6 linear inequalities

Convex Envelopes for Product Terms



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- Meyer and Floudas [2004] derive the facets of the envelopes: for convex envelope, distinguish 9 cases, each giving 5-6 linear inequalities

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

- Cafieri, Lee, and Liberti [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

Vertex-Polyhedral Functions

For a **vertex-polyhedral** function, the convex envelope is determined by the vertices of the box:

Given $f(\cdot)$ vertex-polyhedral over $[\ell, u] \subset \mathbb{R}^n$, value of convex envelope in x is

$$\min_{\lambda \in \mathbb{R}^{2^n}} \left\{ \sum_p \lambda_p f(v^p) \ : \ x = \sum_p \lambda_p v^p, \ \sum_p \lambda_p = 1, \ \lambda \geq 0 \right\} \qquad \text{(C)}$$

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

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The following function classes are vertex-polyhedral:

- Multilinear functions: $f(x) = \sum_{I \in \mathcal{I}} a_I \prod_{i \in I} x_i$, $I \subseteq [n]$ [Rikun, 1997]
- Edge-concave functions: $f(x)$ with $\frac{\partial^2 f}{\partial x_i^2} \leq 0$, $i \in [n]$ [Tardella, 1988/89]

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(C) and (D) allow to compute facets of convex envelope:

- naive: try every subset of $n+1$ vertices: $\binom{2^{n+1}}{n}$ choices!
- Bao, Sahinidis, and Tawarmalani [2009], Meyer and Floudas [2005]: efficient methods for moderate n

α-Underestimators

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

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

$$x^\top Ax + b^\top x + (u_x - x)^\top \operatorname{diag}(\alpha)(x - \ell_x)$$

is a convex underestimator of $x^\top Ax + b^\top x$ w.r.t. the box $[\ell, u]$.

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- can be generalized to twice continuously differentiable functions $g(x)$ by bounding the minimal eigenvalue of the Hessian $\nabla^2 H(x)$ for $x \in [\ell_x, u_x]$ [Androulakis, Maranas, and Floudas, 1995, Adjiman and Floudas, 1996, Adjiman, Dallwig, Floudas, and Neumaier, 1998b]

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- underestimator is exact for $x_i \in \{\ell_i, u_i\}$
- thus, if x is a vector of binary variables ($x_i^2 = x_i$), then

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

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

Eigenvalue Reformulation

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

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

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

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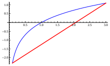
- introducing auxiliary variables $z_i = v_i^\mathsf{T} x$, function becomes separable:

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

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

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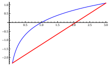
- underestimate concave functions $z_i \mapsto \lambda_i z_i^2$, $\lambda_i < 0$, as known 
- one of the methods for nonconvex QP in CPLEX (keeps convex $\lambda_i z_i^2$ in objective and solves relaxation by QP simplex) [Bliek, Bonami, and Lodi, 2014]

Reformulation Linearization Technique (RLT)

Consider the QCQP

$$\begin{aligned} \min\ & x^{\mathsf{T}} Q_0 x + b_0^{\mathsf{T}} x & & \text{(quadratic)} \\ \text{s.t. } & x^{\mathsf{T}} Q_k x + b_k^{\mathsf{T}} x \le c_k \qquad k = 1, \dots, q & & \text{(quadratic)} \\ & Ax \le b & & \text{(linear)} \\ & \ell \le x \le u & & \text{(linear)} \end{aligned}$$

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\end{aligned}$$

Introduce new variables $X_{i,j} = x_i x_j$:

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\min\ & \langle Q_0, X \rangle + b_0^\top x && && \text{(linear)}\\
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& X = xx^\mathsf{T} & & \text{(quadratic)}
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Adams and Sherali [1986], Sherali and Alameddine [1992], Sherali and Adams [1999]:

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

RLT: Multiplying Bound Constraints

Multiplying bounds $\ell_i \leq x_i \leq u_i$ and $\ell_j \leq x_j \leq u_j$ yields

$$(x_i - \ell_i)(x_j - \ell_j) \geq 0$$
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Multiplying bounds $\ell_i \le x_i \le u_i$ and $\ell_j \le x_j \le u_j$ and using $X_{i,j} = x_i x_j$ yields

$$\begin{aligned}
(x_i - \ell_i)(x_j - \ell_j) \ge 0 \quad &\Rightarrow \quad X_{i,j} \ge \ell_i x_j + \ell_j x_i - \ell_i \ell_j \\
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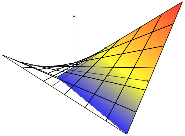

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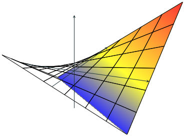

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- the resulting linear relaxation is

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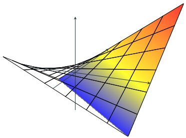

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\end{aligned}$$

- 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:

$$(A_k^\top x - b_k)(x_j - \ell_j) \geq 0 \quad \Rightarrow \quad \sum_{i=1}^{n} A_{k,i} x_i (x_j - \ell_j) - b_k (x_j - \ell_j) \geq 0$$

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ANTIGONE [Misener and Floudas, 2012]:

- linear inequality $(A_k^T x - b_k \leq 0)$ $\times$ variable bound $(x_j - \ell_j \geq 0)$
  $\Rightarrow$ consider for cut generation and bound tightening

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  $\Rightarrow$ consider for cut generation and bound tightening
- linear equality $(A_k^\top x - b_k = 0)$ $\times$ variable (x_j)
  $\Rightarrow$ add to the model (strong cut in context of QAP, pooling, ...)
  (close to bilinear term elimination of Liberti and Pantelides [2006])

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

$$(A_k^\mathsf{T} x - b_k)(x_j - \ell_j) \geq 0 \quad \Rightarrow \quad \sum_{i=1}^{n} A_{k,i}(X_{i,j} - x_i \ell_j) - b_k(x_j - \ell_j) \geq 0$$

$$(A_k^\mathsf{T} x - b_k)(A_{k'}^\mathsf{T} x - b_{k'}) \geq 0 \quad \Rightarrow \quad A_k^\mathsf{T} X A_{k'}^\mathsf{T} - (b_k A_{k'} + b_{k'} A_k^\mathsf{T})x + b_k b_{k'} \geq 0$$

ANTIGONE [Misener and Floudas, 2012]:

- linear inequality $(A_k^T x - b_k \leq 0)$ $\times$ variable bound $(x_j - \ell_j \geq 0)$
  $\Rightarrow$ consider for cut generation and bound tightening
- linear (in)equality $(A_k^T x - b_k {\leq}/{=} 0)$ $\times$ linear (in)equality $(A_{k'}^T x - b_{k'} {\leq}/{=} 0)$
  $\Rightarrow$ consider for cut generation and bound tightening
- linear equality $(A_k^\mathsf{T} x - b_k = 0)$ $\times$ variable (x_j)
  $\Rightarrow$ add to the model (strong cut in context of QAP, pooling, ...)
  (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

Semidefinite Programming (SDP) Relaxation

$$\begin{aligned} \min\ & x^\top Q_0 x + b_0^\top x \\ \text{s.t. } & x^\top Q_k x + b_k^\top x \le c_k \\ & Ax \le b \\ & \ell_x \le x \le u_x \end{aligned} \qquad \Leftrightarrow \qquad \begin{aligned} \min\ & \langle Q_0, X\rangle + b_0^\top x \\ \text{s.t. } & \langle Q_k, X\rangle + b_k^\top x \le c_k \\ & Ax \le b \\ & \ell_x \le x \le u_x \\ & X = xx^\top \end{aligned}$$

- relaxing $X - xx^\top = 0$ to $X - xx^\top \succeq 0$, which is equivalent to

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

yields a semidefinite programming relaxation

Semidefinite Programming (SDP) Relaxation

$$\begin{aligned} \min\ & x^\mathsf{T} Q_0 x + b_0^\mathsf{T} x \\ \text{s.t. } & x^\mathsf{T} Q_k x + b_k^\mathsf{T} x \le c_k \\ & Ax \le b \\ & \ell_x \le x \le u_x \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} \min\ & \langle Q_0, X\rangle + b_0^\mathsf{T} x \\ \text{s.t. } & \langle Q_k, X\rangle + b_k^\mathsf{T} x \le c_k \\ & Ax \le b \\ & \ell_x \le x \le u_x \\ & X = xx^\mathsf{T} \end{aligned}$$

- relaxing $X - xx^\mathsf{T} = 0$ to $X - xx^\mathsf{T} \succeq 0$, which is equivalent to

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

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

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

  is a valid cut that cuts off $\tilde{X}^*$ [Sherali and Fraticelli, 2002]
- available in Couenne and Lindo API (non-default)
- Qualizza, Belotti, and Margot [2009] (Couenne): sparsify cut by setting entries of v to 0

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
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Anstreicher [2012]:

- the SDP relaxation dominates the α-BB underestimators

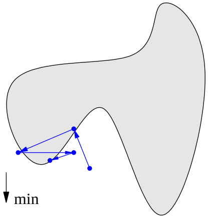
Acceleration – Selected Topics

Primal Heuristics

Sub-NLP Heuristics

Given a solution satisfying all integrality constraints,

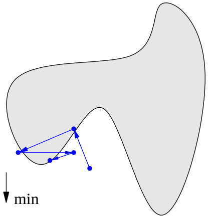
- fix all integer variables in the MINLP
- call an NLP solver to find a local solution to the remaining NLP



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
- variable fixings given by integer-feasible solution to LP relaxation
- additionally, SCIP runs its MIP heuristics on MIP relaxation (rounding, diving, feas. pump, LNS, . . .)



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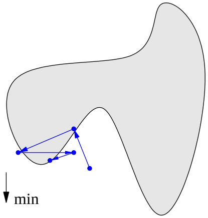

NLP-Diving: solve NLP relaxation, restrict bounds on fractional variable, repeat

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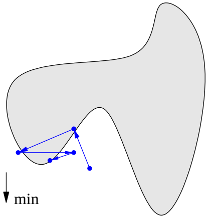


NLP-Diving: solve NLP relaxation, restrict bounds on fractional variable, repeat

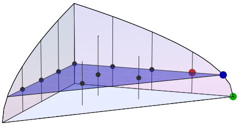
Multistart: run local NLP solver from random starting points to increase likelihood of finding global optimum

Smith, Chinneck, and Aitken [2013]: sample many random starting points, move them cheaply towards feasible region (average gradients of violated constraints), cluster, run NLP solvers from (few) center of cluster (in SCIP [Maher et al., 2017])

Sub-MIP / Sub-MINLP Heuristics

"Undercover" (SCIP) [Berthold and Gleixner, 2014]:

- 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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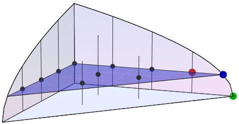
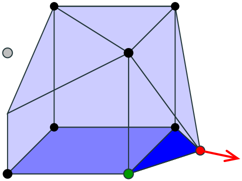


Large Neighborhood Search [Berthold, Heinz, Pfetsch, and Vigerske, 2011]:

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



Iterative Rounding Heuristic (Couenne) [Nannicini and Belotti, 2012]:

1. find a local optimal solution to the NLP relaxation
2. find the nearest integer feasible solution to the MIP relaxation
3. fix integer variables in MINLP and solve remaining sub-NLP locally
4. forbid found integer variable values in MIP relaxation (no-good-cuts) and reiterate

Rounding Heuristics

Iterative Rounding Heuristic (Couenne) [Nannicini and Belotti, 2012]:

1. find a local optimal solution to the NLP relaxation
2. find the nearest integer feasible solution to the MIP relaxation
3. fix integer variables in MINLP and solve remaining sub-NLP locally
4. forbid found integer variable values in MIP relaxation (no-good-cuts) and reiterate

Feasibility Pump (Couenne) [Belotti and Berthold, 2017]:

- 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 NLP and MINLP instances to MINLPLib[1]!

Some recent MINLP reviews:

- Burer and Letchford [2012]
- Belotti, Kirches, Leyffer, Linderoth, Luedtke, and Mahajan [2013]
- Boukouvala, Misener, and Floudas [2016]

Some recent books:

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

[1] http://www.gamsworld.org/minlp/minlplib2/html/index.html

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