An Introduction to Global Optimization of Mixed-Integer Nonlinear Programs

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Outline

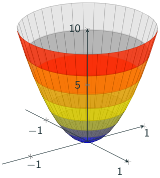
Introduction

Mixed-Integer Nonlinear Programs (MINLPs)

We consider

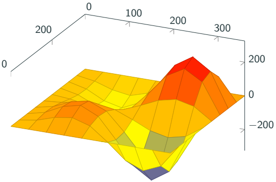
$$\begin{aligned} \min\ & c^\mathsf{T} x \\ \text{s.t. } & g_k(x) \le 0 && \forall k \in [m] \\ & x_i \in \mathbb{Z} && \forall i \in \mathcal{I} \subseteq [n] \\ & x_i \in [\ell_i, u_i] && \forall i \in [n] \end{aligned}$$

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



convex

or



nonconvex

Examples of Mixed-Integer Nonlinearities

- Gas Networks - nonlinear physics for pressure loss in gas pipes, binary decisions on valves, compressor stations



$$Q = 21.87 \frac{T_S}{P_S} \sqrt{\frac{(P_1^2 - P_2^2) D^{5.33}}{T \; L}}$$

- AC power flow - nonlinear function of voltage magnitudes and angles and binary decisions on switching status of power lines

$$p_{ij} = g_{ij} v_i^2 - g_{ij} v_i v_j \cos(\theta_{ij}) + b_{ij} v_i v_j \sin(\theta_{ij})$$

- Circle packing - non-overlap constraints

$$\|x - y\|_2 \geq r_x + r_y$$

- etc.

Applications for MINLP

MINLPLib

A Library of Mixed-Integer and Continuous Nonlinear Programming Instances

This page lists for every application of MINLPLib instances the associated instances.

Agriculture	Alkylation	Argentina utility plant	Asset Management	Autocorrelated Sequences
Batch processing	Breeding	Cascading Tanks	Catalyst Mixing	Catalytic Cracking of Gas Oil
Chain Optimization	Chemical Equilibrium	Coil Compression String Design	Coloring	Computational geometry
Constraint Satisfaction	Cross-dock Door Assignment	Crude Oil Scheduling	Cutting Stock	Cyclic multiproduct scheduling on parallel lines
Cyclic Scheduling of Continuous Parallel Units	Density modification based on single-crystal X-ray diffraction data	Design of Just-in-Time Flowshops	Deterministic Security Constrained Unit Commitment	Edge-crossing minimization in bipartite graphs
Elastic-plastic torsion	Electricity generation	Electricity Networks	Electricity Storage	Electrons on a Sphere
Energy	Facility Location	Farming	Feed Mix	feed plate location
Feed Plate Location	Financial Optimization	four membrane pipe modules in feed-and-bleed coupling	Frequency Assignment	Gas Transmission
Gas Transmission Network Design	Gear Train Design	General Equilibrium	Geometry	Graph Partitioning
Hang Glider	Hanging Chain	Heat Exchanger Network	Heat Integrated Distillation Sequences	Hybrid Dynamic Systems
Hydro Energy System Scheduling	Hydrodealkylation of Toluene	Isometrization	Job Scheduling	Kissing Number Problem
Kriging	Launch Vehicle Design	Layout	Linear Algebra	Location Item Planning
Marine Population Dynamics	Market Equilibrium	Marketing	Matrix Eigenvalues	Max Cut
Methanol to Hydrocarbons	Minimizing Total Average Cycle Stock	Molecular Design	Multi-commodity capacity facility location-allocation	Multi-Product Batch Plant Design
Multiperiod Blend Scheduling	Multiproduct CSTR	Natural Gas Production	Network Design	Neural Networks
Nuclear Reactor Core Reload Pattern	Optimal Control	Optimal vehicle allocation for minimizing greenhouse gas emissions	Parameter estimation in quantitative IR spectroscopy	Particle Steering
Periodic Scheduling of Continuous Multiproduct Plants	Pipeline design	Pooling problem	Pooling Problem	Portfolio Optimization
power plant operation	Process Flowsheets	Process Networks	Process selection	Product Portfolio Optimization
Product positioning in a multiattribute space	Production	pseudo components properties	Pump configuration problem	Quantum Mechanics
Radiation therapy	Rail Line Optimization	Retrofit Planning	Rockets	Sensor Placement
Separation Sequences Based on Distillation	Service System Design	Shape Optimization	Shortest Path	Simultaneous Optimization for HEN Synthesis
Social Accounting Matrix Balancing	Spacecraft Landing	Sports Tournament	Statistics	Structural Optimization
Supply Chain Design with Stochastic Inventory Management	Synthesis of General Distillation Sequences	Synthesis of processing system	Synthesis of Space Truss	Tank Size Design
Telecommunication	Test Problem	Topology Optimization	Traveling Salesman Problem with Neighborhoods	Trim loss minimization problem
Unit Commitment	Waste paper treatment	Waste Water Treatment	Water Network Contamination	Water Network Design
Water Network Operation	Water Resource Management	Winding Factor of Electrical Machines		

(minlplib.org: 1603 instances from 128 applications)

Motivation: Packing Problems

Packing problems are everyday applications for global optimization.

Circle Packing Pavilion at Architectural Institute of Japan (Tokyo, 2012)
https://t-ads.org/blog/2012/11/23/circle-pack-pavilion-at-aij-tokyo/

https://en.neonews.pk/03-May-2018/japanese-pushers-squeeze-in-subway-traveler-video-goes-viral

Let's try out circle packing.

Circle Packing

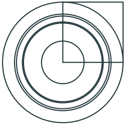
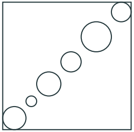
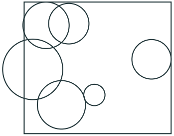
Task: Place N spheres with radii $r_1, \ldots, r_N$ and dimension d in a box of minimal volume.

Formulation: Let $x^i \in \mathbb{R}^d$ be the center of sphere i and $w \in \mathbb{R}^d_+$ define the enclosing box $[0, w]$. Then

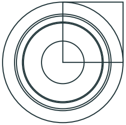
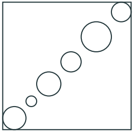
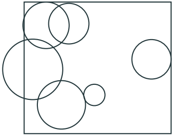
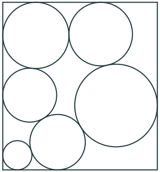
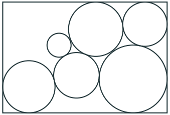
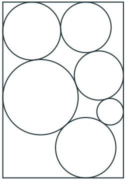
$$
\begin{aligned}
\min \; & \prod_{k=1}^{d} w_k & & \text{(minimize volume)} \\
\text{s.t. } & \|x^i - x^j\|_2 \geq r_i + r_j & 1 \leq i < j \leq N \quad & \text{(spheres do not overlap)} \\
& r_i \leq x^i_k \leq w_k - r_i & i = 1, \ldots, N, k = 1, \ldots, d \quad & \text{(sphere in box)}
\end{aligned}
$$

Consider dimension $d = 2$ (circles) and try some general purpose solvers.

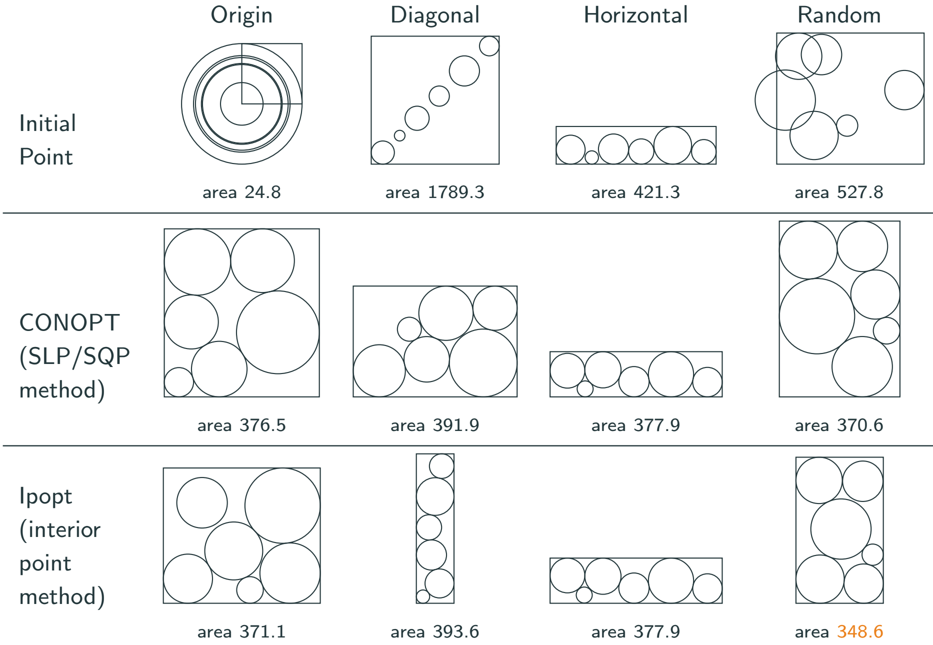
Local NLP Solvers

	Origin	Diagonal	Horizontal	Random
Initial Point				
	area 24.8	area 1789.3	area 421.3	area 527.8

Local NLP Solvers

	Origin	Diagonal	Horizontal	Random
Initial Point	 area 24.8	 area 1789.3	 area 421.3	 area 527.8
CONOPT (SLP/SQP method)	 area 376.5	 area 391.9	 area 377.9	 area 370.6

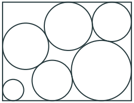
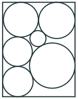
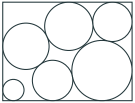
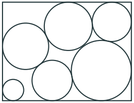
Local NLP Solvers



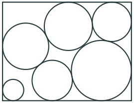
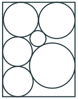
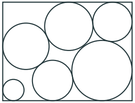
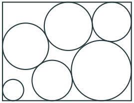
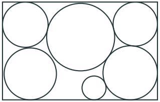
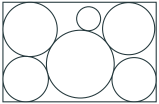
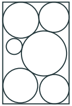
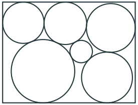
Global Solvers: BARON 25.2.1

Initial Point	Origin 	Diagonal 	Horizontal 	Random 

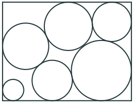
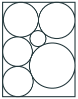
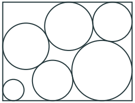
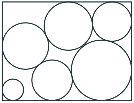
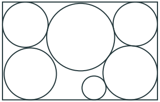
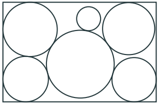
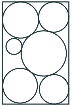
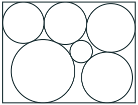
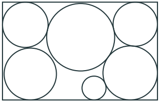
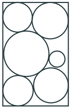
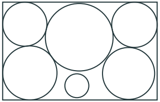
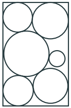
Global Solvers: BARON 25.2.1

Initial Point	Origin 	Diagonal 	Horizontal 	Random 
BARON presolve & init relax. best possible: 99.2	 area: 347.9	 area: 329.9	 area: 347.9	 area: 347.9

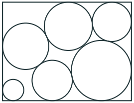
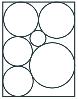
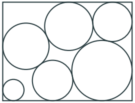
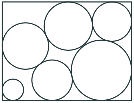
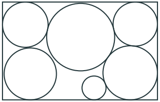
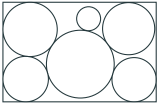
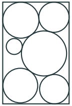
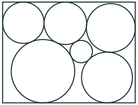
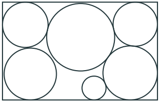
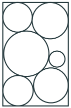
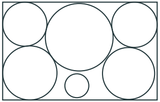
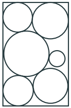
Global Solvers: BARON 25.2.1

Initial Point	Origin	Diagonal	Horizontal	Random
				
BARON presolve & init relax.				
best possible: 99.2	area: 347.9	area: 329.9	area: 347.9	area: 347.9
BARON after 10 seconds				
	area: 327.9 bound: 183.4	area: 329.5 bound: 161.6	area: 329.5 bound: 164.5	area: 330.0 bound: 172.6

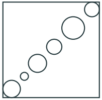
Global Solvers: BARON 25.2.1

Initial Point	Origin	Diagonal	Horizontal	Random
				
BARON presolve & init relax. best possible: 99.2	 area: 347.9	 area: 329.9	 area: 347.9	 area: 347.9
BARON after 10 seconds	 area: 327.9 bound: 183.4	 area: 329.5 bound: 161.6	 area: 329.5 bound: 164.5	 area: 330.0 bound: 172.6
BARON after 60 seconds	 area: 327.9 bound: 286.6	 area: 327.9 bound: 221.6	 area: 327.9 bound: 219.8	 area: 327.9 bound: 270.9

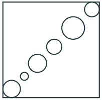
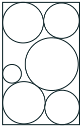
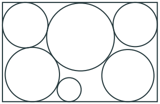
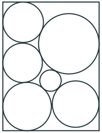
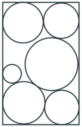
Global Solvers: BARON 25.2.1

Initial Point	Origin 	Diagonal 	Horizontal 	Random 
BARON presolve & init relax. best possible: 99.2	 area: 347.9	 area: 329.9	 area: 347.9	 area: 347.9
BARON after 10 seconds	 area: 327.9 bound: 183.4	 area: 329.5 bound: 161.6	 area: 329.5 bound: 164.5	 area: 330.0 bound: 172.6
BARON after 60 seconds	 area: 327.9 bound: 286.6	 area: 327.9 bound: 221.6	 area: 327.9 bound: 219.8	 area: 327.9 bound: 270.9
proven optimal	time: 81s	time: 115s	time: 115s	time: 77s

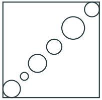
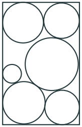
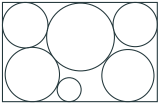
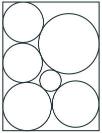
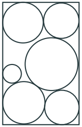
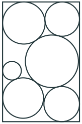
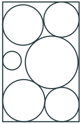
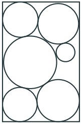
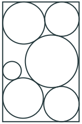
Global Solvers: Gurobi 12.0.1 (1 thread)

Initial	Origin	Diagonal	Horizontal	Random
Gurobi presolve & init relax. bound: 110.6	n/a	 area: 1789.3	 area: 421.3	n/a

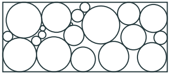
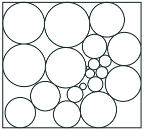
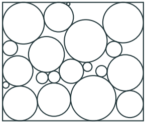
Global Solvers: Gurobi 12.0.1 (1 thread)

Initial	Origin	Diagonal	Horizontal	Random
Gurobi presolve & init relax. bound: 110.6	n/a	 area: 1789.3	 area: 421.3	n/a
Gurobi after 10 seconds	 area: 333.2 bound: 287.3	 area: 331.7 bound: 285.5	 area: 336.7 bound: 276.8	 area: 333.2 bound: 285.3

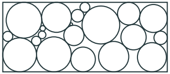
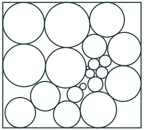
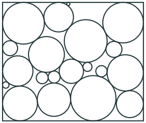
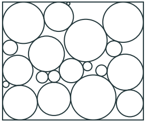
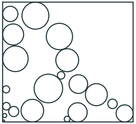
Global Solvers: Gurobi 12.0.1 (1 thread)

Initial	Origin	Diagonal	Horizontal	Random
Gurobi presolve & init relax. bound: 110.6	n/a	 area: 1789.3	 area: 421.3	n/a
Gurobi after 10 seconds	 area: 333.2 bound: 287.3	 area: 331.7 bound: 285.5	 area: 336.7 bound: 276.8	 area: 333.2 bound: 285.3
Gurobi proven optimal	 area: 327.9 time: 26s	 area: 327.9 time: 26s	 area: 327.9 time: 28s	 area: 327.9 time: 25s

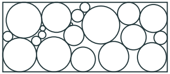
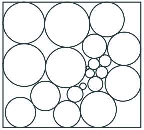
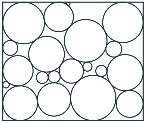
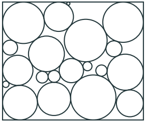
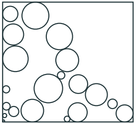
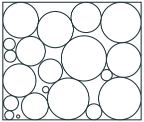
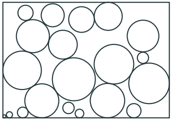
$N = 20$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal	init: origin	init: random	init: random	
			n/a	presolve & init. relax
area: 793.9	area: 840.0	area: 807.4		
		bound: 100.2	bound: 103.8	

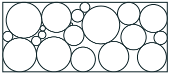
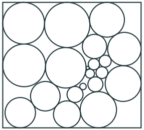
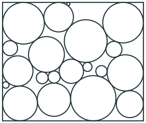
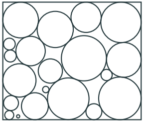
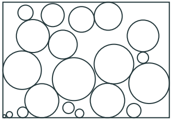
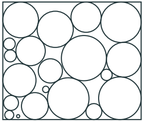
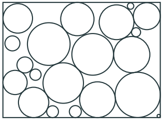
$N = 20$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal  area: 793.9	init: origin  area: 840.0	init: random  area: 807.4 bound: 100.2	init: random n/a bound: 103.8	presolve & init. relax
		 area: 807.4 bound: 100.2	 area: 1900.8 bound: 222.4	after 10 seconds

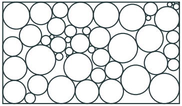
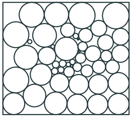
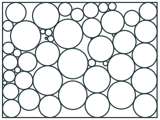
$N = 20$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal  area: 793.9	init: origin  area: 840.0	init: random  area: 807.4 bound: 100.2	init: random n/a bound: 103.8	presolve & init. relax
		 area: 807.4 bound: 100.2	 area: 1900.8 bound: 222.4	after 10 seconds
		 area: 792.7 bound: 102.6	 area: 1034.3 bound: 241.8	after 60 seconds

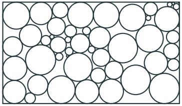
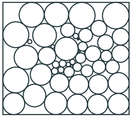
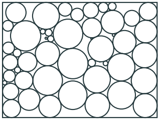
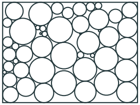
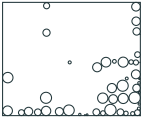
$N = 20$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal  area: 793.9	init: origin  area: 840.0	init: random  area: 807.4 bound: 100.2	init: random n/a bound: 103.8	presolve & init. relax
		 area: 792.7 bound: 102.6	 area: 1034.3 bound: 241.8	after 60 seconds
		 area: 792.7 bound: 156.9	 area: 880.3 bound: 335.4	after 1 hour

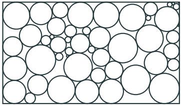
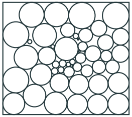
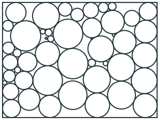
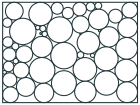
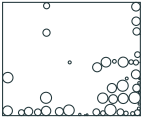
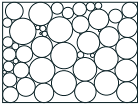
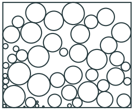
$N = 50$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal	init: origin	init: random	init: random	
			n/a	presolve & init. relax; (same after 10s)
area: 1957.9	area: 2012.0	area: 1931.3		
		bound: 102.3	bound: 101.9	

$N = 50$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal	init: origin	init: random	init: random	presolve & init. relax; (same after 10s)
			n/a	
area: 1957.9	area: 2012.0	area: 1931.3		
		bound: 102.3	bound: 101.9	
				after 60 seconds
		area: 1931.3	area: 12126.4	
		bound: 102.3	bound: 199.0	

$N = 50$ circles

CONOPT	Ipopt	BARON	Gurobi	
init: diagonal	init: origin	init: random	init: random	
			n/a	presolve & init. relax; (same after 10s)
area: 1957.9	area: 2012.0	area: 1931.3		
		bound: 102.3	bound: 101.9	
				after 60 seconds
		area: 1931.3	area: 12126.4	
		bound: 102.3	bound: 199.0	
				after 1 hour
		area: 1931.3	area: 2620.9	
		bound: 109.8	bound: 264.7	

Solving a Mixed-Integer Nonlinear Optimization Problem

Two major tasks:

1. Finding and improving feasible solutions (primal side)
   - Ensure feasibility, sacrifice optimality
   - Important for practical applications
2. Proving optimality (dual side)
   - Ensure optimality, sacrifice feasibility
   - Necessary in order to actually solve the problem

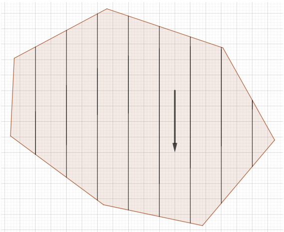
Connected by:

3. Strategy
   - Ensure convergence
   - Divide: branching, decompositions, ...
   - Put together all components

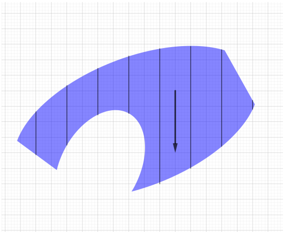
Adding Nonlinearity to a MIP Brings New Challenges

- More numerical issues
- NLP solvers are less efficient and reliable than LP solvers

1. Finding feasible solutions
   - Feasible solutions must also satisfy nonlinear constraints
   - If nonconvex: fixing integer variables and solving the NLP can produce local optima
2. Proving optimality
   - NLP or LP relaxations?
   - If nonconvex: continuous relaxation no longer provides a lower bound
   - "Convenient" descriptions of the feasible set are important
3. Strategy
   - Need to account for all of the above
   - Warmstart for NLP is much less efficient than for LP



→



Solving MINLPs

Convex MINLP:

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

Solving MINLPs

Convex MINLP:

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

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)

Fundamental Methods

Fundamental Methods

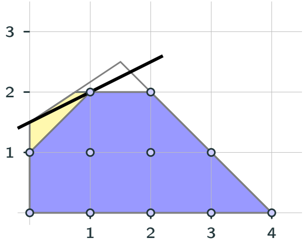
Mixed-Integer Linear Programming

MIP Branch & Cut

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

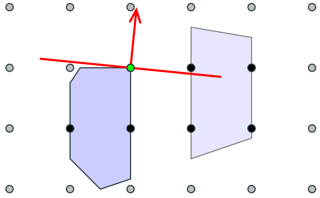
$$\begin{aligned} &\min c^{\mathsf{T}} x, \\ &\text{s.t. } Ax \leq b, \\ &\qquad x_i \in \mathbb{Z}, \quad i \in \mathcal{I}, \end{aligned}$$

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



cutting planes
[Gomory, 1958]

&

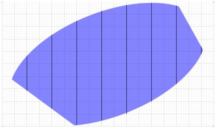


branch-and-bound
[Land and Doig, 1960]

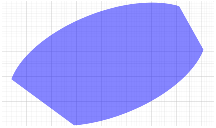
Fundamental Methods

Convex MINLP

NLP relaxation: relax integrality



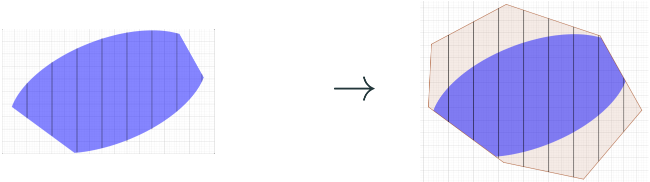
$\longrightarrow$



Relaxations for Convex MINLPs

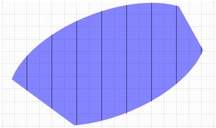
NLP relaxation: relax integrality

MIP relaxation: replace nonlinear set with linear outer approximation

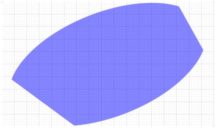


Relaxations for Convex MINLPs

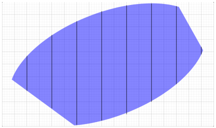
NLP relaxation: relax integrality



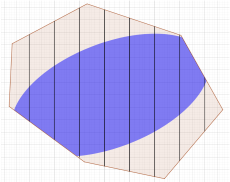
$\longrightarrow$



MIP relaxation: replace nonlinear set with linear outer approximation

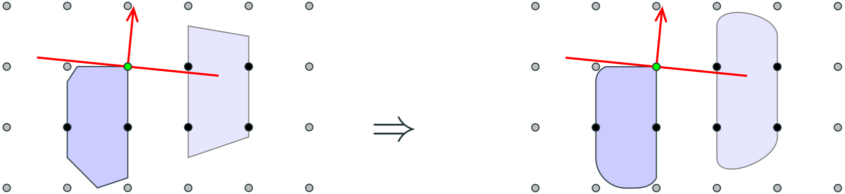


$\longrightarrow$



LP relaxation: relax integrality + linear outer approximation

NLP-based Branch & Bound (NLP-BB)



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 integer variables that take fractional value in NLP solution.

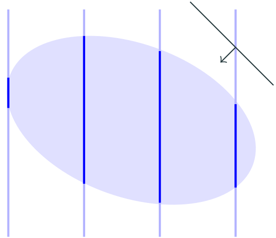
However: Robustness and Warmstarting-capability of NLP solvers not as good as for LP solvers (simplex alg.)

Outer Approximation

Duran and Grossmann [1986]: Replace every nonlinear constraint by linearizations, generated in solution of NLP subproblems obtained by considering any possible fixing for integer variables. Resulting MIP has same optimal value as the MINLP.

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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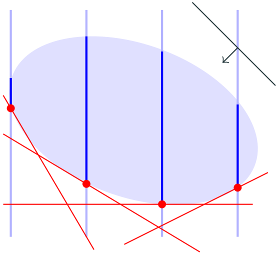

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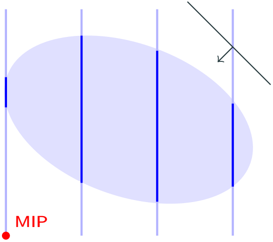

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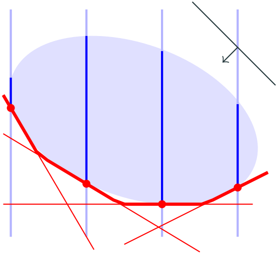

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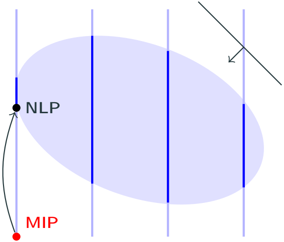

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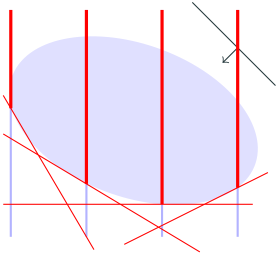

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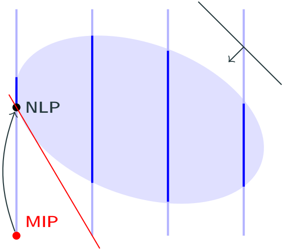

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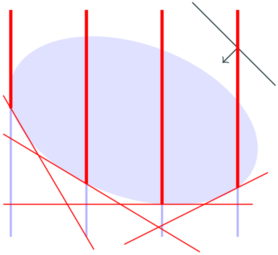

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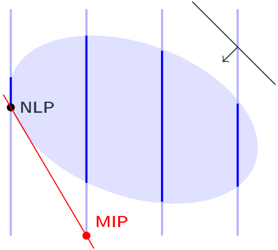

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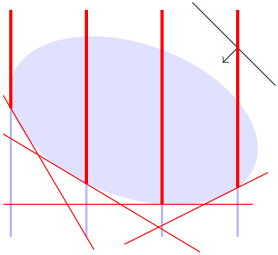

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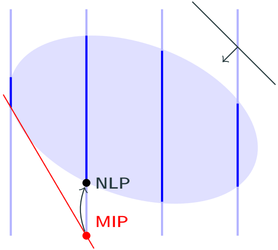

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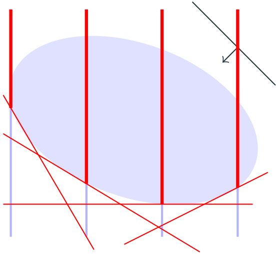

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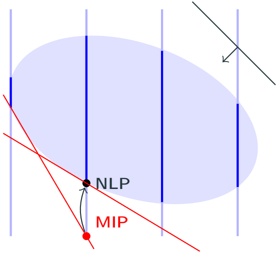

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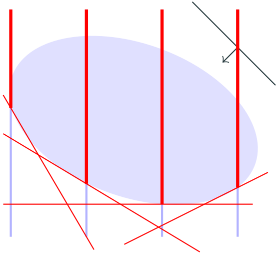

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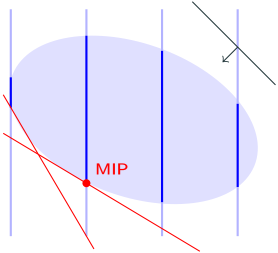


Fundamental Methods

Nonconvex MINLP

Nonconvex MINLP

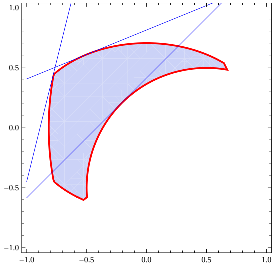
Now: Let some nonlinear constraints be nonconvex.

Outer-Approximation:

- Linearizations may not be valid.

NLP-based Branch & Bound:

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



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Now: Let some nonlinear constraints be nonconvex.

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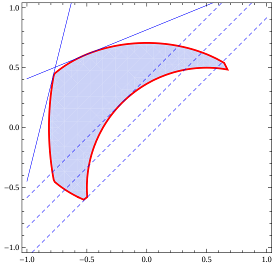

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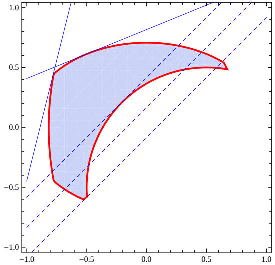
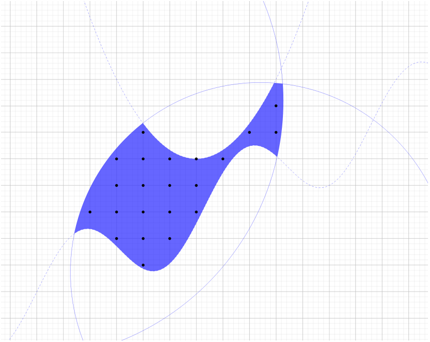


Exact approach: **Spatial Branch & Bound**:

- **Relax nonconvexity** to obtain a tractable relaxation (LP or convex NLP).
- **Branch on "nonconvexities"** to enforce original constraints.

Spatial Branch and Bound

- Solve a relaxation → lower bound
- Run heuristics to look for feasible solutions → upper bound
- Branch on a suitable variable
- Discard parts of the tree that are infeasible or where lower bound > best known upper bound
- Repeat until gap is below given tolerance



Tighter variable bounds → improved relaxations → improved bounds on optimal value.

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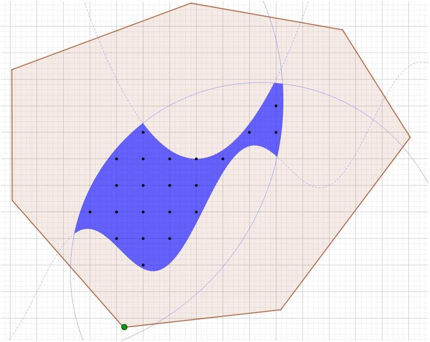

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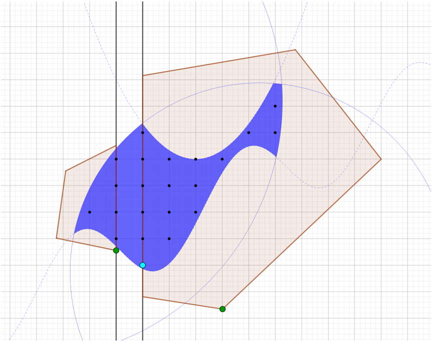

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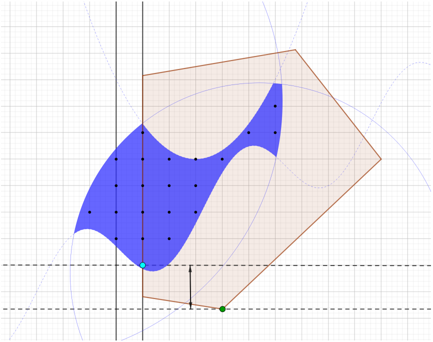

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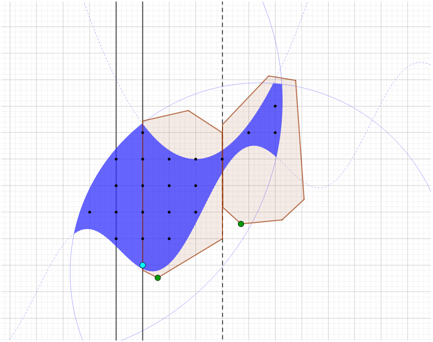

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Convex Relaxation

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

Seek: $\text{conv}(X)$ – convex hull of X

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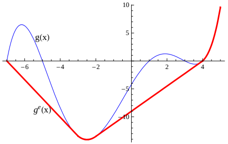

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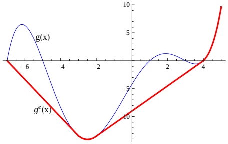

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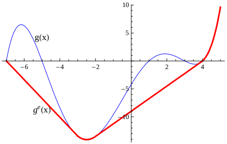
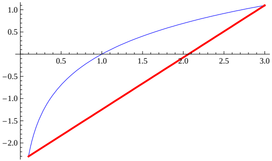


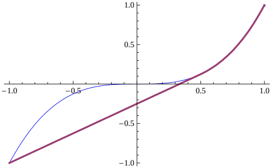
- In practice, convex envelope is not known explicitly in general
  – **except for many “simple functions”**

Convex Envelopes for “simple” functions

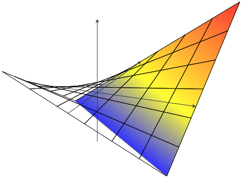
concave functions



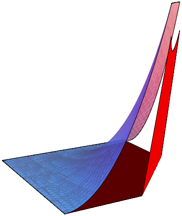
$x^k \quad (k \in 2\mathbb{Z}+1)$



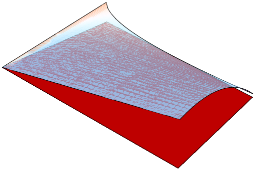
$x \cdot y$



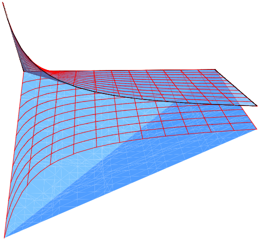
$x^2 \cdot y^2$



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



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



Application to Factorable Functions

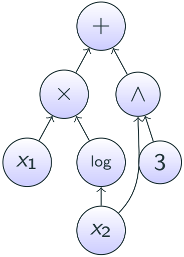
Factorable Functions [McCormick, 1976]

$g(x)$ 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:

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



McCormick [1976] has shown a possibility to compose known envelopes, so convex underestimators for factorable functions can be build.

Reformulation of Factorable MINLP

However, many global solvers reformulate factorable MINLPs by introducing new variables and equations [Smith and Pantelides, 1996, 1997]:

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

- 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., $xyz = (xy)z = x(yz)$.

Spatial Branching

Recall **Spatial Branch & Bound**:

- ✓ **Relax nonconvexity** to obtain a tractable relaxation.
- **Branch on "nonconvexities"** to enforce original constraints.

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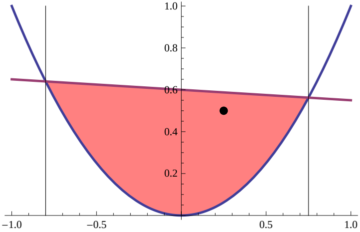
The variable bounds determine the convex relaxation, e.g.,

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



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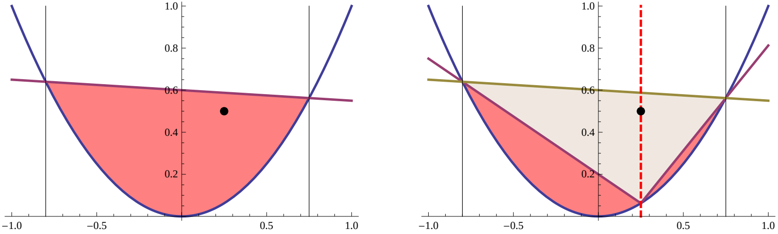
Thus, branching on a nonlinear variable in a nonconvex term allows for tighter relaxations:



Example

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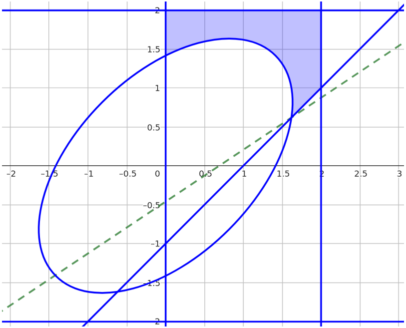
Consider

$$\begin{aligned} \text{minimize} \quad & -2x + 3y \\ \text{such that } & x^2 - xy + y^2 \geq 2 \\ & x - y \leq 1 \\ & x \in [0, 2], \\ & y \in [-2, 2] \end{aligned}$$



Optimal solution:

- from the picture, both inequalities are active $\Rightarrow y = x - 1$

$\Rightarrow 2 = x^2 - x(x-1) + (x-1)^2 = x^2 - x + 1 \Rightarrow (x - \frac{1}{2})^2 = \frac{5}{4}$

- $x \geq 0 \Rightarrow x = \frac{1+\sqrt{5}}{2}$, $y = \frac{\sqrt{5}-1}{2}$, objective $= \frac{\sqrt{5}-5}{2} \approx -1.38$

Example: Solvers

Solve with general purpose solvers (GAMS 49.2.0):

$$\begin{aligned} \min \; & -2x + 3y \\ \text{s.t. } & x^2 - xy + y^2 \geq 2 \\ & x - y \leq 1 \\ & x \in [0, 2], \\ & y \in [-2, 2] \end{aligned}$$

solver	optimum	time	B&B tree
ANTIGONE	-1.381966	0.03s	1 node
BARON	-1.381966	0.04s	1 node
CONOPT3	infeasible	0.01s	–
CONOPT4	-1.381966	0.01s	–
Gurobi	-1.381966	0.02s	9 nodes
Ipopt	infeasible	0.02s	–
Knitro	-1.381966	0.02s	–
Lindo API	fail	0.02s	–
Minos	infeasible	0.01s	–
SCIP	-1.381966	0.08s	1 node
SNOPT	infeasible	0.01s	–
XPRESS	-1.381966	0.10s	31 nodes

Initial LP Relaxation: X enters the stage

Constraint:

$$x^2 - xy + y^2 \geq 2, \qquad x \in [0, 2], \qquad y \in [-2, 2]$$

Introduce $X_{xx} = x^2$, $X_{xy} = xy$, $X_{yy} = y^2$.

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Since x^2 and y^2 are convex, we can use a tangent and secant on its graph, e.g.,

$$\underbrace{4 + 4(x-2)}_{\text{tangent at } x=2} \leq x^2 \leq \underbrace{0 + \frac{4-0}{2-0}(x-0)}_{\text{secant from } x=0 \text{ to } x=2} \quad \Rightarrow \quad 4x - 4 \leq X_{xx} \leq 2x$$

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$$\underbrace{4 + 4(x-2)}_{\text{tangent at } x=2} \leq x^2 \leq \underbrace{0 + \frac{4-0}{2-0}(x-0)}_{\text{secant from } x=0 \text{ to } x=2} \quad \Rightarrow \quad 4x - 4 \leq X_{xx} \leq 2x$$

Or derive inequalities by multiplying variable bound constraints:

$$0 \leq (x-0)^2 \qquad = x^2 \qquad = X_{xx} \qquad \rightarrow X_{xx} \geq 0$$

Initial LP Relaxation: X enters the stage

Constraint:

$$x^2 - xy + y^2 \geq 2, \qquad x \in [0, 2], \qquad y \in [-2, 2]$$

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Or derive inequalities by multiplying variable bound constraints:

$$\begin{array}{llll} 0 \leq (x-0)^2 & = x^2 & = X_{xx} & \rightarrow X_{xx} \geq 0 \\ 0 \leq (2-x)^2 & = x^2 - 4x + 4 & = X_{xx} - 4x + 4 & \rightarrow X_{xx} \geq 4x - 4 \end{array}$$

Initial LP Relaxation: X enters the stage

Constraint:

$$x^2 - xy + y^2 \geq 2, \qquad x \in [0,2], \qquad y \in [-2,2]$$

Introduce $X_{xx} = x^2$, $X_{xy} = xy$, $X_{yy} = y^2$.

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Or derive inequalities by multiplying variable bound constraints:

$$\begin{array}{llll}
0 \leq (x-0)^2 & = x^2 & = X_{xx} & \to X_{xx} \geq 0 \\
0 \leq (2-x)^2 & = x^2 - 4x + 4 & = X_{xx} - 4x + 4 & \to X_{xx} \geq 4x - 4 \\
0 \leq (2-x)(x-0) & = -x^2 + 2x & = -X_{xx} + 2x & \to X_{xx} \leq 2x
\end{array}$$

Initial LP Relaxation: X enters the stage

Constraint:

$$x^2 - xy + y^2 \geq 2, \qquad x \in [0,2], \qquad y \in [-2,2]$$

Introduce $X_{xx} = x^2$, $X_{xy} = xy$, $X_{yy} = y^2$.

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Or derive inequalities by multiplying variable bound constraints:

$$\begin{array}{llll}
0 \leq (x-0)^2 & = x^2 & = X_{xx} & \to X_{xx} \geq 0 \\
0 \leq (2-x)^2 & = x^2 - 4x + 4 & = X_{xx} - 4x + 4 & \to X_{xx} \geq 4x - 4 \\
0 \leq (2-x)(x-0) & = -x^2 + 2x & = -X_{xx} + 2x & \to X_{xx} \leq 2x \\
0 \leq (y-(-2))^2 & = y^2 + 4y + 4 & = X_{yy} + 4y + 4 & \to X_{yy} \geq -4y - 4 \\
0 \leq (y-(-2))(2-y) & = -y^2 + 4 & = -X_{yy} + 4 & \to X_{yy} \leq 4 \\
0 \leq (2-y)^2 & = y^2 - 4y + 4 & = X_{yy} - 4y + 4 & \to X_{yy} \geq 4y - 4 \\
0 \leq (x-0)(y-(-2)) & = xy + 2x & = X_{xy} + 2x & \to X_{xy} \geq -2x \\
0 \leq (x-0)(2-y) & = -xy + 2x & = -X_{xy} + 2x & \to X_{xy} \leq 2x \\
0 \leq (2-x)(y-(-2)) & = -xy - 2x + 2y + 4 & = -X_{xy} - 2x + 2y + 4 & \to X_{xy} \leq -2x + 2y + 4 \\
0 \leq (2-x)(2-y) & = xy - 2x - 2y + 4 & = X_{xy} - 2x - 2y + 4 & \to X_{xy} \geq 2x + 2y - 4
\end{array}$$

Initial LP Relaxation

Replace $(x^2,\ xy,\ y^2)$ by (X_{xx}, X_{xy}, X_{yy}) and add derived inequalities:

$$\min\ -2x + 3y$$

$$\text{s.t. } \cancel{x^2 - xy + y^2 \geq 2}$$

$$X_{xx} - X_{xy} + X_{yy} \geq 2$$

$$x - y \leq 1$$

$$X_{xx} \geq 4x - 4$$

$$X_{xx} \leq 2x$$

$$X_{yy} \geq -4y - 4$$

$$X_{yy} \geq 4y - 4$$

$$X_{xy} \leq 2x$$

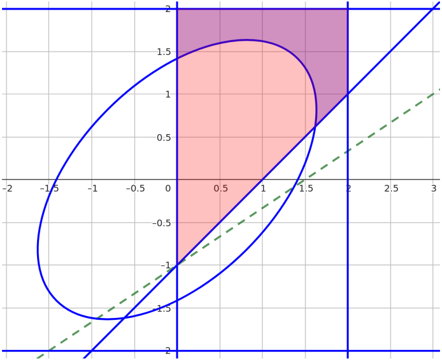
$$X_{xy} \leq -2x + 2y + 4$$

$$X_{xy} \geq 2x + 2y + 4$$

$$x \in [0, 2], y \in [-2, 2]$$

$$X_{xx} \in [0, \infty], X_{yy} \in [-\infty, 4]$$

Projected on (x, y):

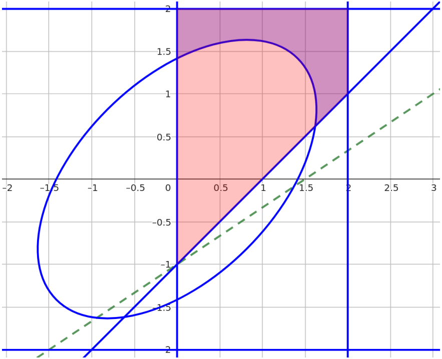


- Lower Bound = -3

$\Rightarrow$ none of the inequalities in (X_{xx}, X_{xy}, X_{yy}) are active :-(

Tighten variable bounds

- inequalities for relaxation were derived using bounds on x and y
- tighter bounds could mean a tighter relaxation



Tighten variable bounds

- inequalities for relaxation were derived using bounds on x and y
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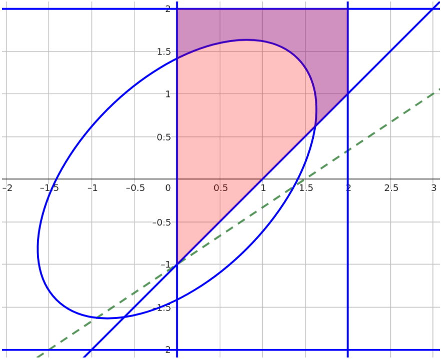
$$x - y \leq 1, x \in [0, 2] \quad \Rightarrow y \geq x - 1 \geq -1$$

$$x - y \leq 1, y \in [-2, 2] \quad \Rightarrow x \leq y + 1 \leq 3$$



- updated bounds:

$$x \in [0, 2], \quad y \in [-1, 2]$$

Tighten variable bounds

- inequalities for relaxation were derived using bounds on x and y
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$$x - y \leq 1, x \in [0, 2] \quad \Rightarrow y \geq x - 1 \geq -1$$
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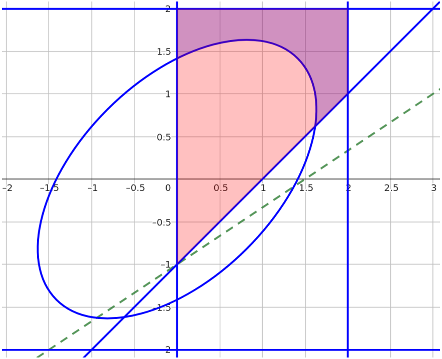
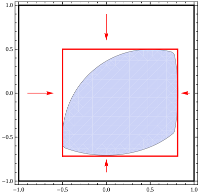


- updated bounds:

$$x \in [0, 2], \quad y \in [-1, 2]$$

- from $x^2 - xy + y^2 \geq 2$, no bound tightening can be derived

In General: 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

Feasibility-Based Bound Tightening

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 $\Rightarrow$ used for "probing"

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

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

Linear Constraints:

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

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

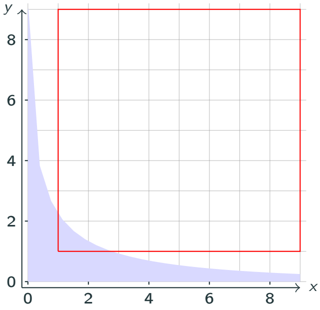
$$x_j \geq \frac{1}{a_j} \begin{cases} b - \sum_{i:a_i>0, i\neq j} a_i u_i - \sum_{i:a_i<0} a_i \ell_i, & \text{if } a_j > 0 \\ c - \sum_{i:a_i>0} a_i \ell_i - \sum_{i:a_i<0, i\neq j} a_i u_i, & \text{if } a_j < 0 \end{cases}$$

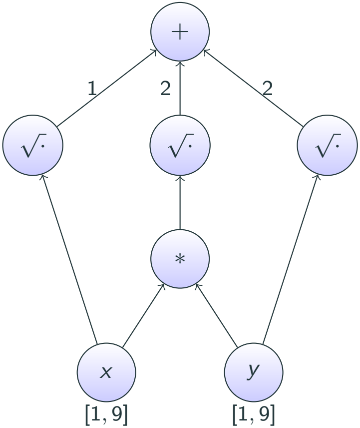
- Belotti, Cafieri, Lee, and Liberti [2010]: fixed point of iterating FBBT on set of linear constraints can be computed by solving one LP

Example:

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

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





Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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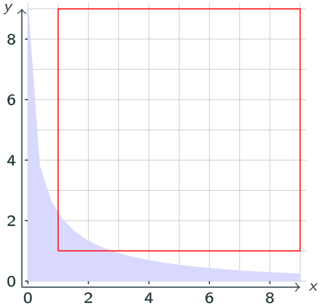
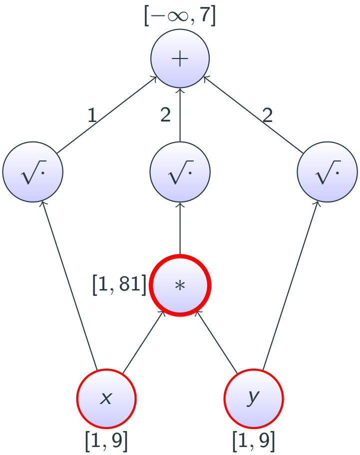


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)



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

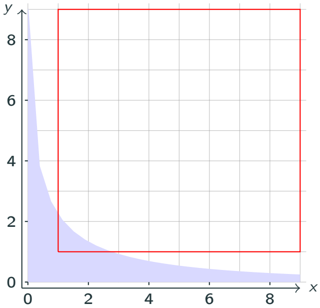
Application of **Interval Arithmetics** [Moore, 1966]

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:

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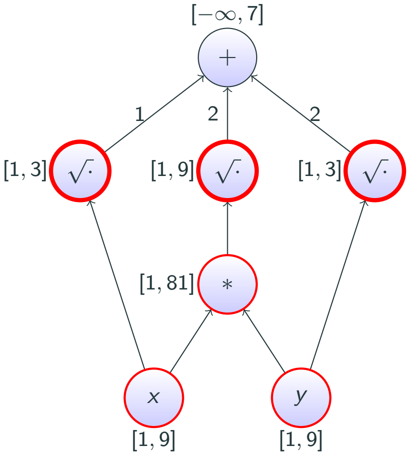


$\sqrt{[1,9]} = [1,3]$ $\quad$ $\sqrt{[1,81]} = [1,9]$

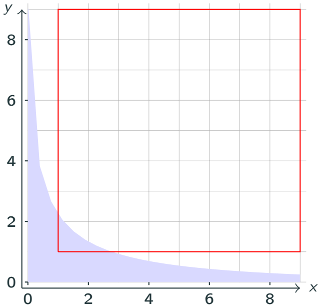
Application of **Interval Arithmetics** [Moore, 1966]

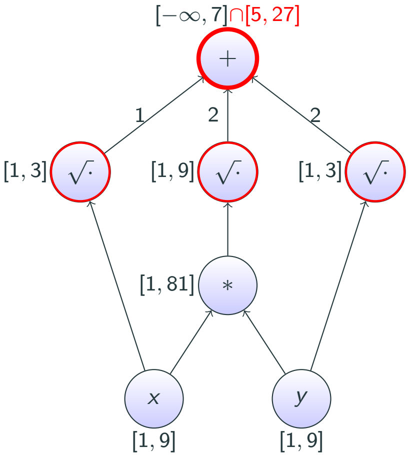
Feasibility-Based Bound Tightening on Expression Tree

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)

$$[1, 3] + 2\,[1, 9] + 2\,[1, 3] = [5, 27]$$

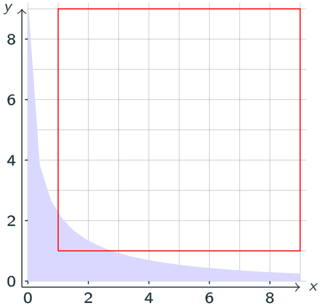
Application of **Interval Arithmetics** [Moore, 1966]

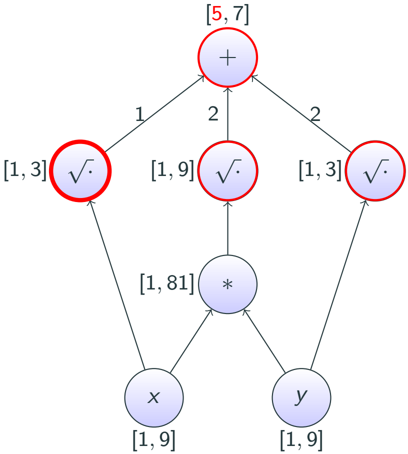
Feasibility-Based Bound Tightening on Expression Tree

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)

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

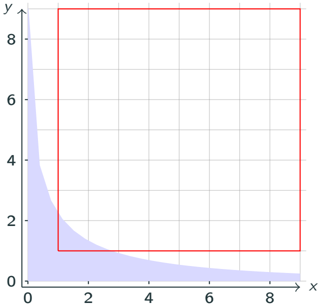
Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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



Forward propagation:

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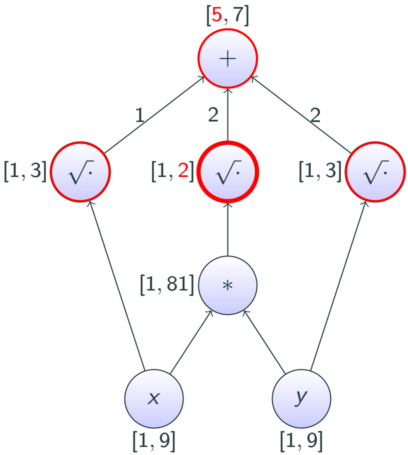

$$([5, 7] - [1, 3] - 2\,[1, 3])/2 = [-2, 2]$$

Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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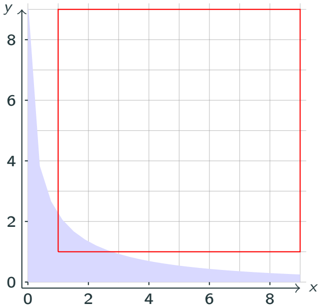

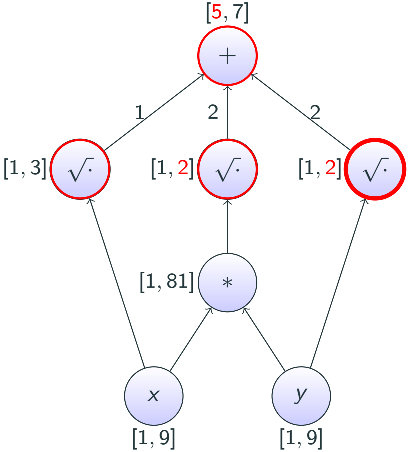

$([5, 7] - [1, 3] - 2\,[1, 2])/2 = [-1, 2]$

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

Application of **Interval Arithmetics** [Moore, 1966]

Example:

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

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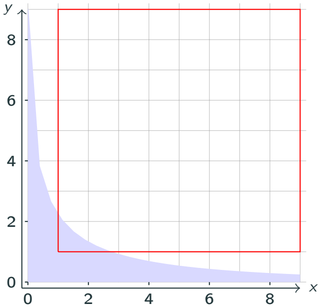

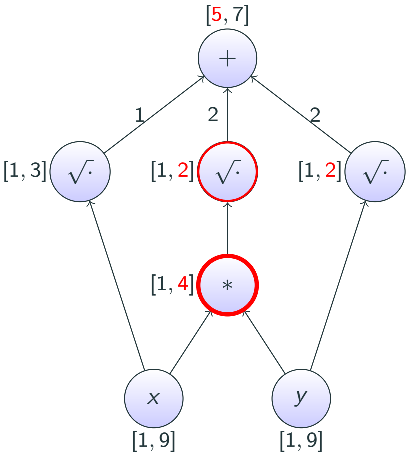

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

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

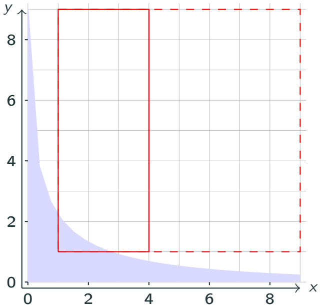
Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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

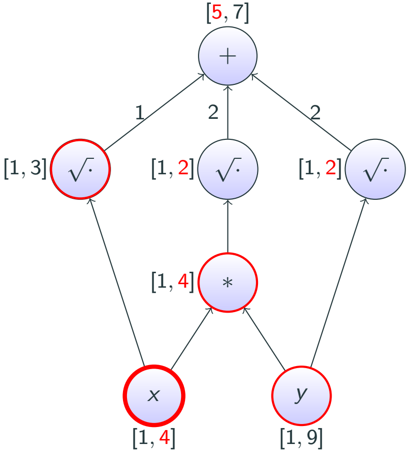


Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)



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

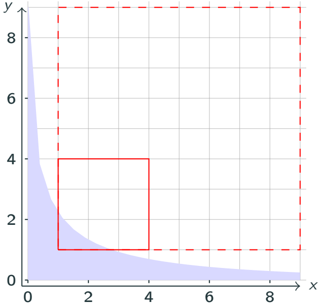
Application of **Interval Arithmetics** [Moore, 1966]

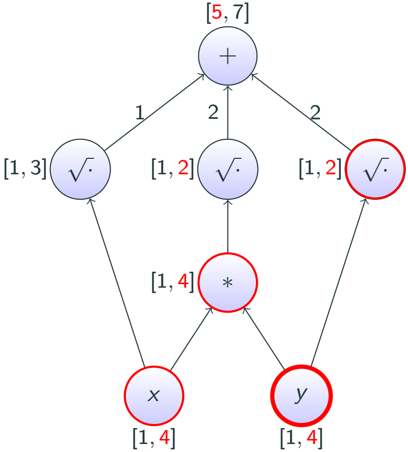
Feasibility-Based Bound Tightening on Expression Tree

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)

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

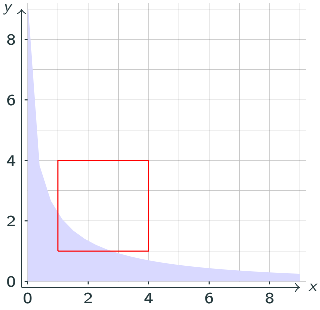
Application of **Interval Arithmetics** [Moore, 1966]

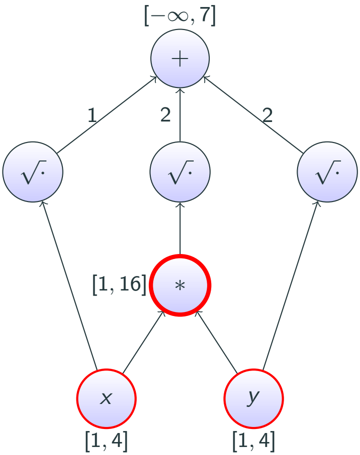
Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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





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

Forward propagation:

- compute bounds on intermediate nodes (bottom-up)

Backward propagation:

- reduce bounds using reverse operations (top-down)

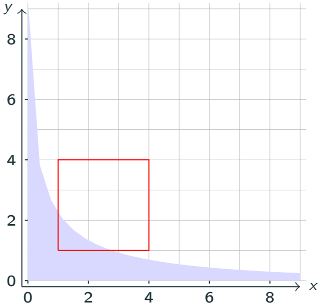
Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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



Forward propagation:

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Backward propagation:

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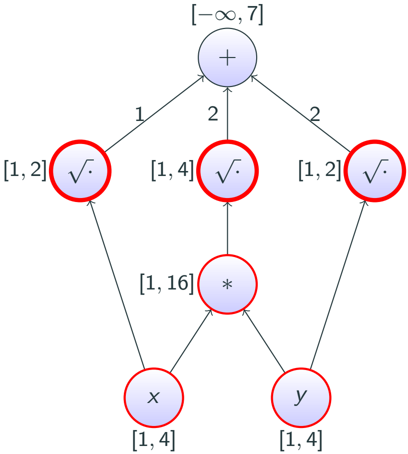


$$\sqrt{[1,4]} = [1,2] \qquad \sqrt{[1,16]} = [1,4]$$

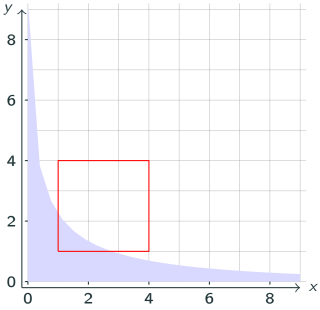
Application of **Interval Arithmetics** [Moore, 1966]

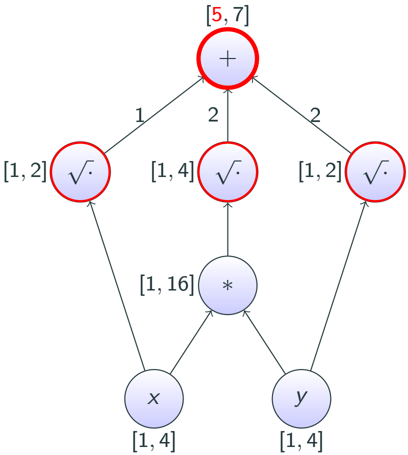
Feasibility-Based Bound Tightening on Expression Tree

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)

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

Backward propagation:

- reduce bounds using reverse operations (top-down)

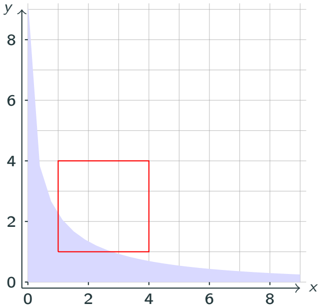
Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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



Forward propagation:

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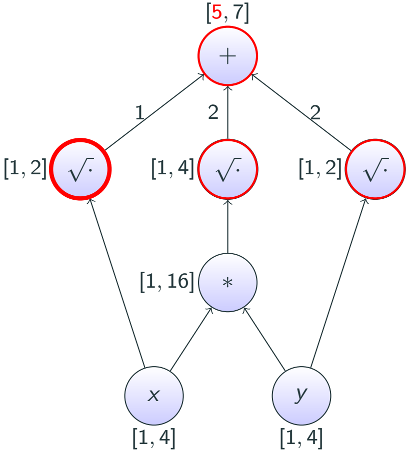


$$[5, 7] - 2\,[1, 4] - 2\,[1, 2] = [-7, 3]$$

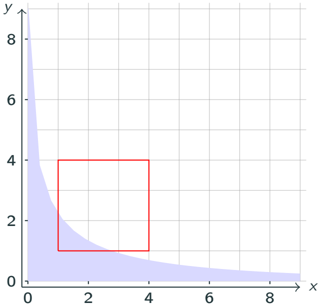
Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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

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

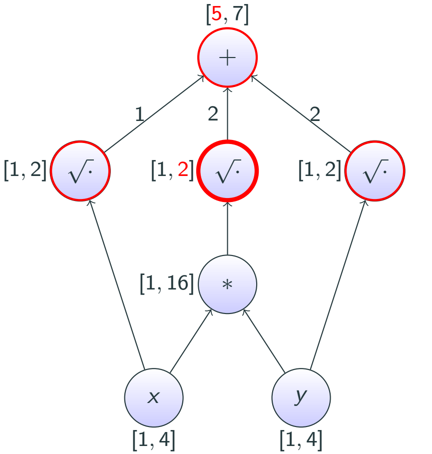


Forward propagation:

- 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]

Feasibility-Based Bound Tightening on Expression Tree

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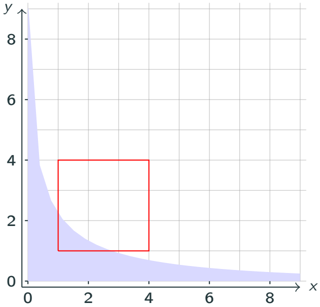

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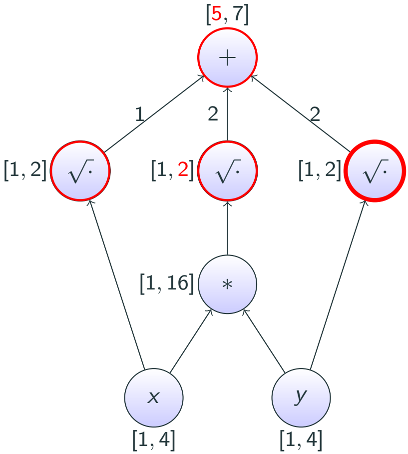

$$([5, 7] - [1, 2] - 2\,[1, 4])/2 = [-2.5, 2]$$

Application of **Interval Arithmetics** [Moore, 1966]

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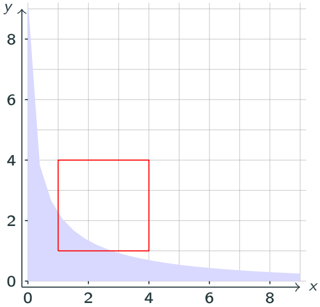

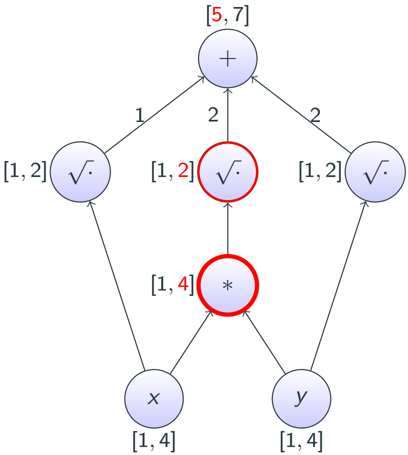

$[1,2]^2 = [1,4]$

Forward propagation:

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Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

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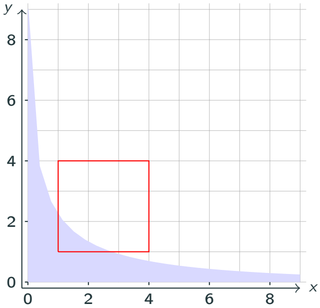

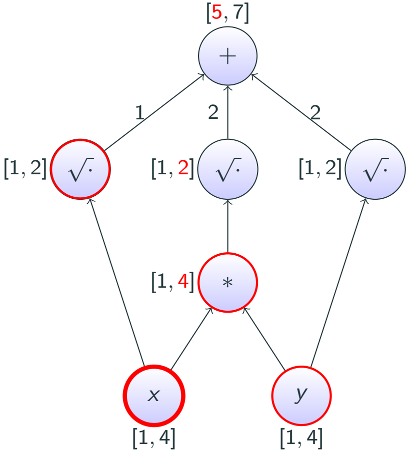

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$[1, 2]^2 = [1, 4]$ $\quad$ $[1, 4]/[1, 4] = [1/4, 4]$

Application of **Interval Arithmetics** [Moore, 1966]

Feasibility-Based Bound Tightening on Expression Tree

Example:

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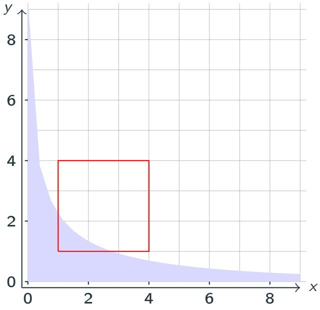
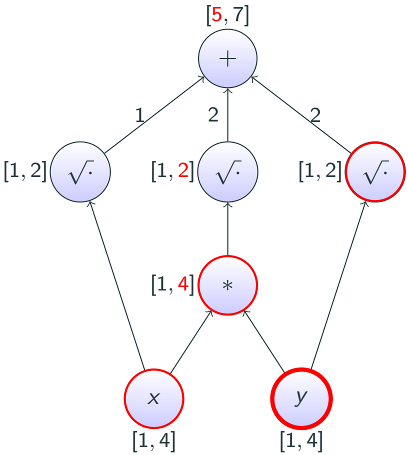
$$x, y \in [1, 4]$$





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

Forward propagation:

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Application of **Interval Arithmetics** [Moore, 1966]

Problem: Overestimation

Back to Example: Relaxation after bound update

Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\ x - y \leq 1,\ x \in [0,2], y \in [-1, 2]\}$

Linearization: $x^2 \to X_{xx},\ xy \to X_{xy},\ y^2 \to X_{yy}$

Recompute initial relaxation with lower bound on y updated to -1:

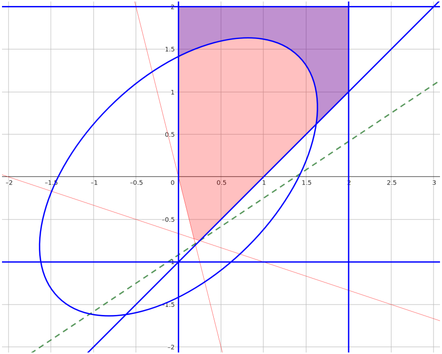
$$
\begin{aligned}
0 &\leq (x-0)^2 &&= x^2 &&= X_{xx} &&\to X_{xx} \geq 0\\
0 &\leq (2-x)^2 &&= x^2 - 4x + 4 &&= X_{xx} - 4x + 4 &&\to X_{xx} \geq 4x - 4\\
0 &\leq (2-x)(x-0) &&= -x^2 + 2x &&= -X_{xx} + 2x &&\to X_{xx} \leq 2x\\
0 &\leq (y-(-1))^2 &&= y^2 + y + 1 &&= X_{yy} + y + 1 &&\to X_{yy} \geq -y - 1\\
0 &\leq (y-(-1))(2-y) &&= -y^2 + y + 2 &&= -X_{yy} + y + 2 &&\to X_{yy} \leq y + 2\\
0 &\leq (2-y)^2 &&= y^2 - 4y + 4 &&= X_{yy} - 4y + 4 &&\to X_{yy} \geq 4y - 4\\
0 &\leq (x-0)(y-(-1)) &&= xy + x &&= X_{xy} + x &&\to X_{xy} \geq -x\\
0 &\leq (x-0)(2-y) &&= -xy + 2x &&= -X_{xy} + 2x &&\to X_{xy} \leq 2x\\
0 &\leq (2-x)(y-(-1)) &&= -xy - x + 2y + 2 &&= -X_{xy} - x + 2y + 2 &&\to X_{xy} \leq -x + 2y + 2\\
0 &\leq (2-x)(2-y) &&= xy - 2x - 2y + 4 &&= X_{xy} - 2x - 2y + 4 &&\to X_{xy} \geq 2x + 2y - 4
\end{aligned}
$$

LP Relaxation after Bound Tightening

With $y \geq -1$:

$$
\begin{aligned}
\min\ & -2x + 3y \\
\text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\
& x - y \leq 1 \\
& X_{xx} \geq 0 \\
& X_{xx} \geq 4x - 4 \\
& X_{xx} \leq 2x \\
& X_{yy} \geq -y - 1 \\
& X_{yy} \leq y + 2 \\
& X_{yy} \geq 4y - 4 \\
& X_{xy} \geq -x \\
& X_{xy} \leq 2x \\
& X_{xy} \leq -x + 2y + 2 \\
& X_{xy} \geq 2x + 2y + 4 \\
& x \in [0, 2], y \in [-1, 2]
\end{aligned}
$$

Projected on (x, y):



- Lower Bound = -2.75 (improvement from -3)

Can we get more cuts?

- we should make use of the inequality $x - y \leq 1$
- Idea: multiply bounds with linear inequality

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$$
\begin{aligned}
0 &\leq (1 - x + y)(x - 0) &&= x - x^2 + xy &&= x - X_{xx} + X_{xy} \\
0 &\leq (1 - x + y)(2 - x) &&= 2 - x - 2x + x^2 + 2y - xy &&= 2 - 3x + X_{xx} + 2y - X_{xy}
\end{aligned}
$$

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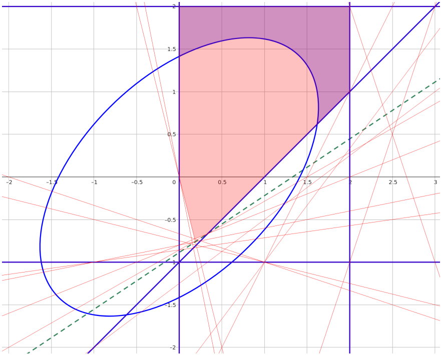
0 &\leq (1-x+y)(2-x) &&= 2 - x - 2x + x^2 + 2y - xy &&= 2 - 3x + X_{xx} + 2y - X_{xy} \\
0 &\leq (1-x+y)(y-(-1)) &&= y + 1 - xy - x + y^2 + y &&= 2y + 1 - X_{xy} - x + X_{yy} \\
0 &\leq (1-x+y)(2-y) &&= 2 - y - 2x + xy + 2y - y^2 &&= 2 + y - 2x + X_{xy} - X_{yy}
\end{aligned}
$$

Inequalities that couple several X $\rightarrow$ looks promising

LP Relaxation with additional cuts

$$\begin{aligned}
\min\ & -2x + 3y \\
\text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\
& x - y \leq 1 \\
& X_{xx} \geq 0 \\
& X_{xx} \geq 4x - 4 \\
& X_{xx} \leq 2x \\
& X_{yy} \geq -y - 1 \\
& X_{yy} \leq y + 2 \\
& X_{yy} \geq 4y - 4 \\
& X_{xy} \geq -x \\
& X_{xy} \leq 2x \\
& X_{xy} \leq -x + 2y + 2 \\
& X_{xy} \geq 2x + 2y + 4 \\
& X_{xx} - X_{xy} \leq x \\
& X_{xx} - X_{xy} \geq 3x - 2y - 2 \\
& X_{xy} - X_{yy} \leq 2y - x + 1 \\
& X_{xy} - X_{yy} \geq 2x - y - 2 \\
& x \in [0, 2], y \in [-1, 2]
\end{aligned}$$

Projected on (x, y):



- Lower Bound = -2.66 (improvement from -2.75)

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& X_{xy} \leq 2x \\
& X_{xy} \leq -x + 2y + 2 \\
& X_{xy} \geq 2x + 2y + 4 \\
& X_{xx} - X_{xy} \leq x \\
& X_{xx} - X_{xy} \geq 3x - 2y - 2 \\
& X_{xy} - X_{yy} \leq 2y - x + 1 \\
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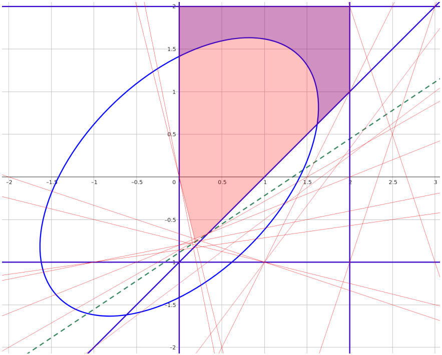

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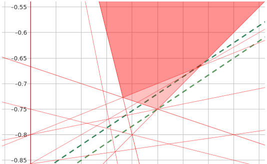

In General: Reformulation Linearization Technique (RLT)

Consider the QCQP

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

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

$$\begin{aligned}
\min\ & \langle Q_0, X \rangle + b_0^\top x && && \text{(linear)}\\
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& Ax \le b && && \text{(linear)}\\
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& X = xx^\top && && \text{(quadratic)}
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\min\ & x^\mathsf{T} Q_0 x + b_0^\mathsf{T} x && && \text{(quadratic)}\\
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& \ell \le x \le u && && \text{(linear)}\\
& X = xx^\mathsf{T} && && \text{(quadratic)}
\end{aligned}$$

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

$$
\begin{aligned}
(x_i - \ell_i)(x_j - \ell_j) &\geq 0 \\
(x_i - u_i)(x_j - u_j) &\geq 0 \\
(x_i - \ell_i)(x_j - u_j) &\leq 0 \\
(x_i - u_i)(x_j - \ell_j) &\leq 0
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RLT: Multiplying Bound Constraints

Multiplying bounds $\ell_i \leq x_i \leq u_i$ and $\ell_j \leq x_j \leq u_j$ and using $X_{i,j} = x_i x_j$ yields

$$(x_i - \ell_i)(x_j - \ell_j) \geq 0 \quad \Rightarrow \quad X_{i,j} \geq \ell_i x_j + \ell_j x_i - \ell_i \ell_j$$

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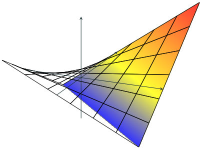

- these are more widely known as McCormick inequalities [McCormick, 1976]

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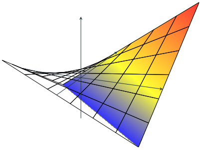

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- the resulting linear relaxation is

$$\begin{aligned}
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& Ax \le b, \quad \ell \le x \le u \\
& X_{i,j} \ge \ell_i x_j + \ell_j x_i - \ell_i \ell_j \qquad i,j = 1,\dots,n, i \le j \\
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\end{aligned}$$

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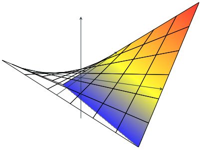

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- these inequalities are used by all solvers
- not every solver introduces $X_{i,j}$ variables explicitly

RLT: Multiplying Bounds and Inequalities

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

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

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

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

RLT: Multiplying Bounds and Inequalities

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

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

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

RLT is also used for polynomial programs [Sherali and Tuncbilek, 1992]:

- any monomial $\prod_i x_i^{\alpha_i}$ is replaced by a new variable
- more than two bounds or (in)equalities are multiplied
- solver: RAPOSa [González-Rodríguez et al., 2022]

Back to Example: Objective Cutoff

$\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\ x - y \leq 1,\ x \in [0,2], y \in [-1,2]\}$

Assume the optimal solution with objective $= \frac{\sqrt{5}-5}{2}$ has been found, e.g., by a NLP solver, but proof of optimality is still missing.

Objective cutoff: Look only for improving solutions: $-2x + 3y \leq \frac{\sqrt{5}-5}{2}$

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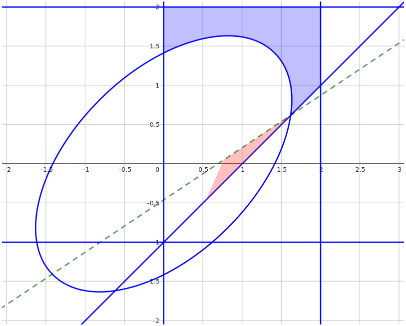
RLT with this inequality:

$$0 \leq 2X_{xx} - 3X_{xy} + \frac{\sqrt{5}}{2}x - \frac{5}{2}x$$

$$0 \leq -2X_{xx} + 3X_{xy} - \frac{\sqrt{5}}{2}x + \frac{13}{2}x - 6y + \sqrt{5} - 5$$

$$0 \leq 2X_{xy} - 3X_{yy} + \frac{\sqrt{5}}{2}y + 2x - \frac{11}{2}y + \frac{\sqrt{5}}{2} - \frac{5}{2}$$

$$0 \leq -2X_{xy} + 3X_{yy} - \frac{\sqrt{5}}{2}y + 4x - \frac{7}{2}y + \sqrt{5} - 5$$



- Lower bound = -2.46
  (improvement from -2.66)

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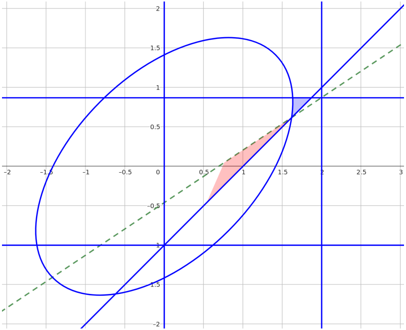

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Use objective cutoff for bound tightening: $y \leq \frac{1}{3}\left(\frac{\sqrt{5}-5}{2} + 2x\right) \leq \frac{\sqrt{5}+3}{6} \approx 0.87$

More Bound Tightening

Looking at the LP relaxation including objective cutoff only, it seems that variable bounds could be improved further:

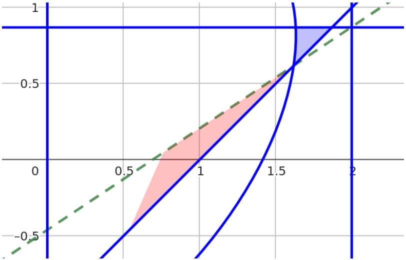
$$x - y \leq 1$$

$$-2x + 3y \leq \frac{\sqrt{5} - 5}{2}$$

$$\dots$$

$$x \in [0, 2],\ y \in [-1, 0.87]$$

Apparently, $x \ll 2$.



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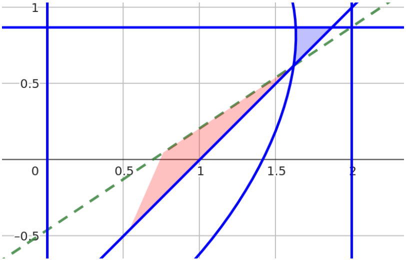

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Propagating each inequality individually works:

$$x - y \leq 1 \Rightarrow x \leq 1.87$$
$$-2x + 3y \leq -1.38 \Rightarrow y \leq 0.79$$
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Belotti [2013]: FBBT on two linear constraints simultaneously

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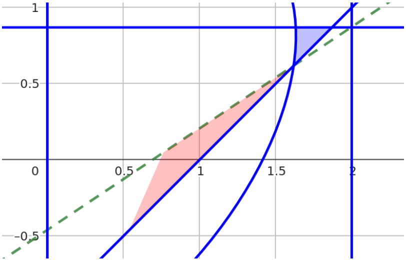

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Eventually, this terminates with upper bounds equal to

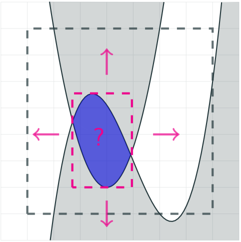
$$\max\{x : x - y \leq 1, -2x + 3y \leq -1.38\}$$
$$\max\{y : x - y \leq 1, -2x + 3y \leq -1.38\}$$

Idea: Just solve this LP!

Belotti [2013]: FBBT on two linear constraints simultaneously

In General: 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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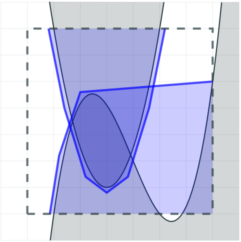
Optimization-based Bound Tightening [Quesada and Grossmann, 1993, Maranas and Floudas, 1997, Smith and Pantelides, 1999, . . .]:

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



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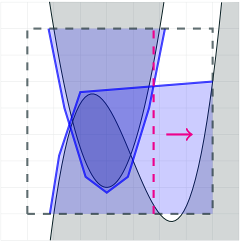

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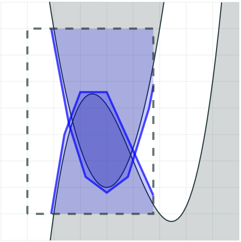

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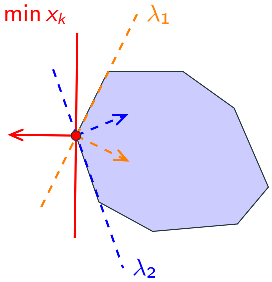

Advanced implementation [Gleixner, Berthold, Müller, and Weltge, 2017]:

- 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

Back to Example: Bound Tightening by OBBT

We tightened upper bounds via

$$\max\left\{x : x - y \leq 1, -2x + 3y \leq \frac{\sqrt{5}-5}{2}\right\} = \frac{1+\sqrt{5}}{2} \approx 1.62$$

$$\max\left\{y : x - y \leq 1, -2x + 3y \leq \frac{\sqrt{5}-5}{2}\right\} = \frac{\sqrt{5}-1}{2} \approx 0.62$$

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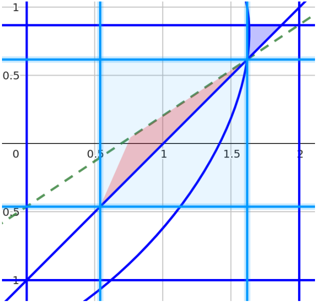
To tighten also lower bounds, consider the complete relaxation:

$$\begin{aligned}
&\min x \text{ or } y \\
&\text{s.t. } x - y \le 1 \\
&\quad -2x + 3y \le \frac{\sqrt{5}-5}{2} \\
&\quad X_{xx} - X_{xy} + X_{yy} \ge 2 \\
&\quad \text{RLT}(X, x, y), \\
&\quad x \in \left[0, \frac{1+\sqrt{5}}{2}\right], y \in \left[-1, \frac{\sqrt{5}-1}{2}\right]
\end{aligned}$$

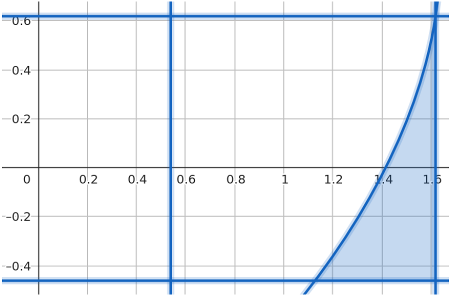


$\Rightarrow x \ge 0.54,\ y \ge -0.46$

FBBT on quadratic constraint

With the tighter bounds from OBBT, let us try to derive further boundtightening from the quadratic constraint, that is

$$\min / \max\{x \text{ or } y \;:\; x^2 - xy + y^2 \geq 2, x \in [0.54, 1.62], y \in [-0.46, 0.62]\}$$



For y we cannot expect any tightening, but what about the lower bound for x?

FBBT on quadratic constraint – do the math

$x^2 - xy + y^2 = (y - \frac{1}{2}x)^2 + \frac{3}{4}x^2$ is supposed to be ≥ 2

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$$\Rightarrow x \in \left(\left[-\infty, \frac{1}{2}y - \sqrt{2 - \frac{3}{4}y^2}\right] \cup \left[\frac{1}{2}y + \sqrt{2 - \frac{3}{4}y^2}, \infty\right]\right) \cap [0.54, 1.62]$$

The right-hand side now depends on y only.

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The right-hand side now depends on y only.

We now need to find

$$\max_{y \in [-0.46, 0.62]} \frac{1}{2}y - \sqrt{2 - \frac{3}{4}y^2} \qquad \min_{y \in [-0.46, 0.62]} \frac{1}{2}y + \sqrt{2 - \frac{3}{4}y^2}$$

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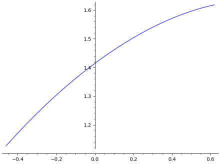
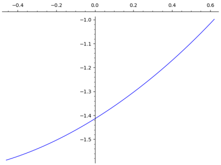
These are univariate bound-constrained optimization problems.





FBBT on quadratic constraint – do the math (cont.)

$$\max_{y\in[-0.46,0.62]} \frac{1}{2}y - \sqrt{2-\frac{3}{4}y^2} \underbrace{=}_{y=0.62} \frac{0.62}{2} - \sqrt{2-\frac{3}{4}0.62^2} \approx -1$$

$$\min_{y\in[-0.46,0.62]} \frac{1}{2}y + \sqrt{2-\frac{3}{4}y^2} \underbrace{=}_{y=-0.46} -\frac{0.46}{2} + \sqrt{2-\frac{3}{4}(-0.46)^2} \approx 1.13$$

FBBT on quadratic constraint – do the math (cont.)

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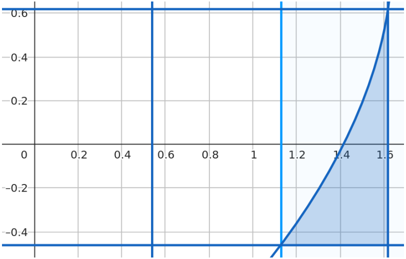
$$\Rightarrow x \in \left(\left[-\infty, \underbrace{\frac{1}{2}y - \sqrt{2-\frac{3}{4}y^2}}_{\approx -1}\right] \cup \left[\underbrace{\frac{1}{2}y + \sqrt{2-\frac{3}{4}y^2}}_{\approx 1.13}, \infty\right]\right) \cap [0.54, 1.62] = [1.13, 1.62]$$



Note: feasible range on x is disconnected (2 intervals); we used $x \geq 0.54$ to exclude the left interval and derive $x \geq 1.13$

Vigerske and Gleixner [2017]: general formulas

Updated Relaxation after FBBT and OBBT

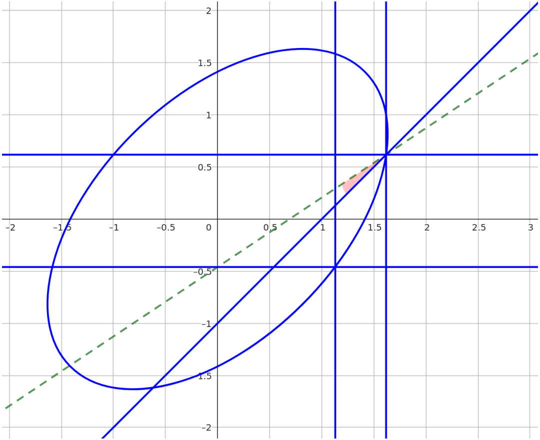
We derived

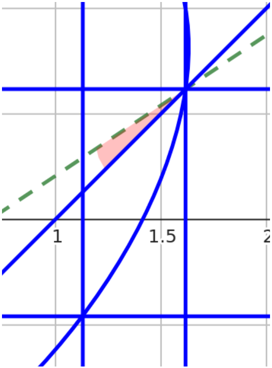
- $x \le 1.62$, $y \le 0.62$ via OBBT or alternating FBBT on $x - y \le 1$ and $-2x + 3y \le -1.38$
- $y \ge -0.46$ via OBBT on LP relaxation (incl. RLT cuts)
- $x \ge 1.13$ via <u>careful</u> (avoid overestimation of interval arith.) FBBT on $x^2 - xy + y^2 \ge 2$

Update RLT:

$$
\begin{aligned}
&0 \le (x - 1.13)^2 && 0 \le (x - 1.13)(1 - x + y)\\
&0 \le (1.62 - x)^2 && 0 \le (1.62 - x)(1 - x + y)\\
&0 \le (x - 1.13)(1.62 - x) && 0 \le (y + 0.46)(1 - x + y)\\
& && 0 \le (0.62 - y)(1 - x + y)\\
&0 \le (y + 0.46)^2 && \\
&0 \le (0.62 - y)^2 && 0 \le (x - 1.13)(-1.38 + 2x - 3y)\\
&0 \le (0.62 - y)(y + 0.46) && 0 \le (1.62 - x)(-1.38 + 2x - 3y)\\
& && 0 \le (y + 0.46)(-1.38 + 2x - 3y)\\
&0 \le (x - 1.13)(y + 0.46) && 0 \le (0.62 - y)(-1.38 + 2x - 3y)\\
&0 \le (x - 1.13)(0.62 - y) && \\
&0 \le (1.62 - x)(y + 0.46) && xx \to X_{xx},\ xy \to X_{xy},\ yy \to X_{yy}\\
&0 \le (1.62 - x)(0.62 - y) &&
\end{aligned}
$$

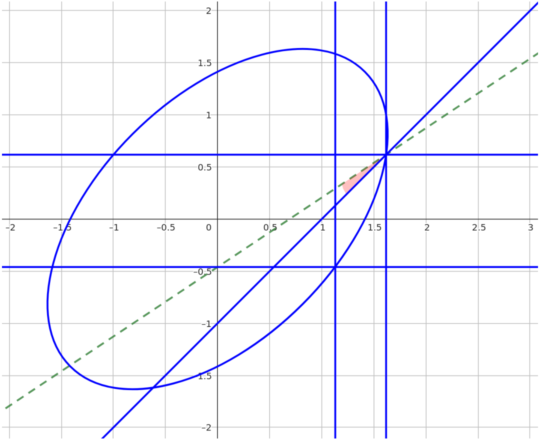
Updated Relaxation (cont.)

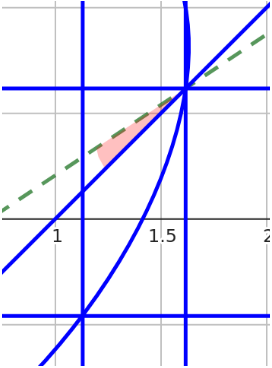




Lower bound = -1.76 (improvement from -2.46, optimal value = -1.38)

Updated Relaxation (cont.)





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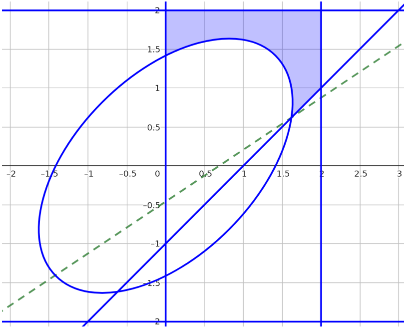
Next steps:

- OBBT improves lower bound on y due to tighter RLT cuts
- FBBT on quad. cons. improves lower bound on x due to better bound on y
- RLT cuts tighten due to better lower bounds on x and y

Recap

Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\, x - y \leq 1,\, x \in [0, 2], y \in [-2, 2]\}$



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Problem: $\min\{-2x+3y \;:\; x^2 - xy + y^2 \geq 2,\, x - y \leq 1,\, x \in [0,2], y \in [-2,2]\}$

Initial Relaxation:

- replace any square and bilinear term by new variable (X)
- derive cuts for X by multiplying variable bounds, e.g., $(2-x)(2-y) \geq 0$ (also known as McCormick cuts)

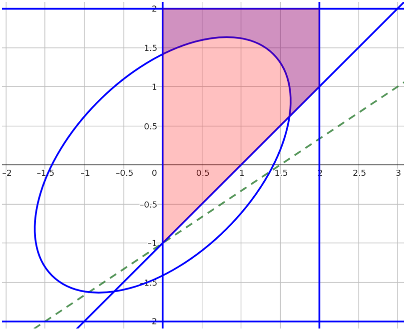
LP Relaxation:

$$\min \; -2x + 3y$$
$$\text{s.t. } X_{xx} - X_{xy} + X_{yy} \geq 2$$
$$x - y \leq 1$$

RLT(multiply bounds)

$x \in [0,2]$

$y \in [-2,2]$



Lower bound = -3

Recap

Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\ x - y \leq 1,\ x \in [0,2], y \in [-2,2]\}$

Bound Tightening:

- FBBT on linear constraint: $x - y \leq 1 \Rightarrow y \geq -1$

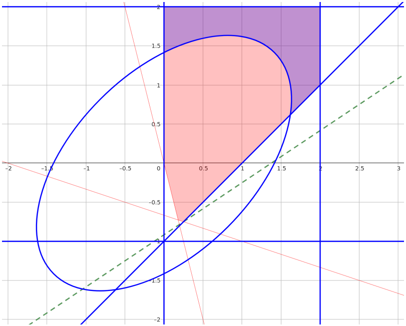
LP Relaxation:

$$\begin{aligned} \min \ & -2x + 3y \\ \text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\ & x - y \leq 1 \end{aligned}$$

RLT(multiply bounds)

$x \in [0,2]$

$y \in [-1,2]$



Lower bound = -2.75

Recap

Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\ x - y \leq 1,\ x \in [0, 2], y \in [-2, 2]\}$

RLT with Linear Inequality:

- multiply $x - y \leq 1$ with variable bound, e.g., $(2 - x)(1 - x + y) \geq 0$

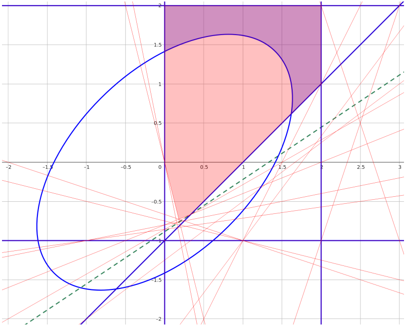
LP Relaxation:

$$\min \ -2x + 3y$$
$$\text{s.t. } X_{xx} - X_{xy} + X_{yy} \geq 2$$
$$x - y \leq 1$$

RLT(bounds & $x - y \leq 1$)

$x \in [0, 2]$

$y \in [-1, 2]$



Lower Bound = -2.66

Recap

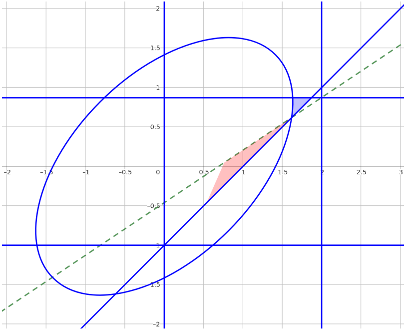
Problem: $\min\{-2x+3y \;:\; x^2 - xy + y^2 \geq 2,\, x-y \leq 1,\, x \in [0,2], y \in [-2,2]\}$

Objective Cutoff:

- look only for improving solutions: $-2x+3y \leq -1.36$
- use for FBBT and RLT (improving upper bound can improve lower bound!)

LP Relaxation:

$$\begin{aligned}
\min\ & -2x+3y \\
\text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\
& x - y \leq 1 \\
& -2x + 3y \leq 1.38 \\
& \text{RLT(bounds \& linear inequ.)} \\
& x \in [0,2] \\
& y \in [-1, 0.87]
\end{aligned}$$



Lower Bound = -2.46

Recap

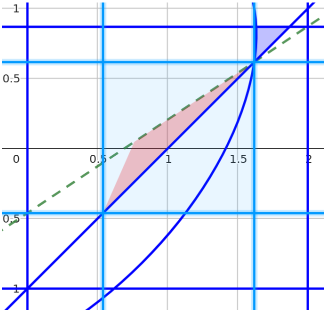
Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2, \ x - y \leq 1, \ x \in [0,2], y \in [-2,2]\}$

Bound Tightening:

- OBBT on relaxation: min / max x or y w.r.t. LP relaxation
- expensive, best when objective cutoff included

LP Relaxation:

$$\begin{aligned} \min \ & -2x + 3y \\ \text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\ & x - y \leq 1 \\ & -2x + 3y \leq 1.38 \\ & \text{RLT(bounds \& linear inequ.)} \\ & x \in [0.54, 1.62] \\ & y \in [-0.46, 0.62] \end{aligned}$$



Recap

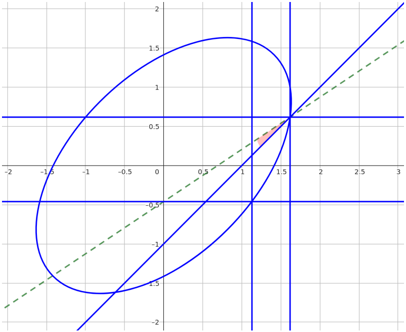
Problem: $\min\{-2x + 3y \ : \ x^2 - xy + y^2 \geq 2,\ x - y \leq 1,\ x \in [0, 2], y \in [-2, 2]\}$

Bound Tightening:

- FBBT on $x^2 - xy + y^2 \geq 2 \Rightarrow x \geq 1.13$

LP Relaxation:

$$\begin{aligned} \min \ & -2x + 3y \\ \text{s.t. } & X_{xx} - X_{xy} + X_{yy} \geq 2 \\ & x - y \leq 1 \\ & -2x + 3y \leq 1.38 \\ & \text{RLT(bounds \& linear inequ.)} \\ & x \in [1.13, 1.62] \\ & y \in [-0.46, 0.62] \end{aligned}$$



Lower bound = -1.76

Further Techniques

Further Techniques

Dual Side (Tighter Relaxations)

Semidefinite Programming (SDP) Relaxation

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

- 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
- Anstreicher [2009]: the SDP and RLT relaxations do not dominate each other; combining both can produce substantially better bounds

SDP Cuts

SDP is computationally demanding, so approximate by linear inequalities:

- for $\tilde{X}^* \not\succeq 0$ compute eigenvector v with eigenvalue $\lambda < 0$, then

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

  is a valid cut that cuts off $\tilde{X}^*$ [Sherali and Fraticelli, 2002]

- these cuts can be very dense (involve many variables), which slows down the LP solver

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Approaches for sparser cuts:

- Qualizza et al. [2009]: relax cut by setting entries of v to 0
- Saxena et al. [2011]: project into x-variables space (no X variables in cut)
- Sherali et al. [2012]: consider only a subset of variables and corresponding submatrix of X
  - Baltean-Lugojan et al. [2018]: pick submatrix via neural network
  - SCIP [Bestuzheva et al., 2021]: consider only two variables and corresponding 2×2 submatrix of X

Second Order Cones (SOC)

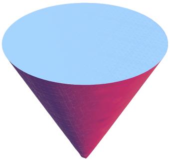
Consider a constraint $\quad x^{\mathsf{T}}Ax + b^{\mathsf{T}}x \leq c.$

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

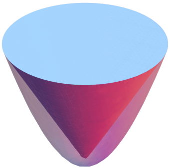
$$\sum_{k=1}^{N} x_k^2 - x_{N+1}^2 \leq 0, x_{N+1} \geq 0 \qquad \Leftrightarrow \qquad \sqrt{\sum_{k=1}^{N} x_k^2} \leq x_{N+1}$$

- $\sqrt{\sum_{k=1}^{N} x_k^2}$ is a convex term that can easily be linearized

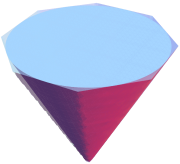
Example: $x^2 + y^2 - z^2 \leq 0$ in $[-1,1] \times [-1,1] \times [0,1]$



feasible region



not recognizing SOC



recognizing SOC

(initial relaxation)

Cone Disaggregation

For high-dimensional cones (large N), linearizations of $\sqrt{\sum_{k=1}^{N} x_k^2}$ generate dense cuts $\Rightarrow$ slow LP solves.

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Vielma et al. [2016]: consider disaggregated formulation in extended space:

- introduce new variables z_k, $k = 1, \dots, N$ and add constraints

$$z_k \geq \frac{x_k^2}{x_{N+1}}, \qquad \sum_{k=1}^{N} z_k \leq x_{N+1}$$

- then SOC $\sum_k x_k^2 \leq x_{N+1}^2$ is satisfied because

$$\frac{1}{x_{N+1}} \sum_{k=1}^{N} x_k^2 \leq \sum_{k=1}^{N} z_k \leq x_{N+1}$$

- new cons. $x_k^2/x_{N+1} \leq z_k$ are 3-dimensional SOC:

$$x_k^2 \leq z_k x_{N+1} = 1/4\left((z_k + x_{N+1})^2 - (z_k - x_{N+1})^2\right)$$

$$\Leftrightarrow \sqrt{4x_k^2 + (z_k - x_{N+1})^2} \leq z_k + x_{N+1}$$

$\Downarrow$

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 et al., 2009, Vigerske, 2013]

Analyze Expression for Hessian: Klaus, Merk, Wiedom, Laue, and Giesen [2022]

Stronger relaxations with semi-continuous variables

Consider

$$x^2 \le w, \qquad \ell y \le x \le uy, \quad y \in \{0,1\}, \qquad \text{(with } \ell > 0\text{)}.$$

That is, $x \in \{0\} \cup [\ell, u]$.

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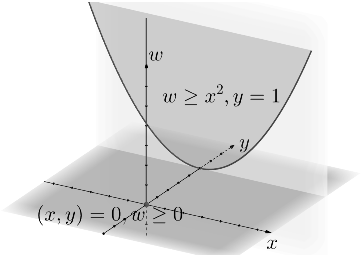
A tight relaxation would be the convex hull of relaxations for $y = 0$ and $y = 1$:

$$\text{conv}\left(\underbrace{\{(0,w,0) \;:\; w \ge 0\}}_{y=0} \;\cup\; \underbrace{\{(x,w,1) \;:\; x^2 \le w, x \in [\ell, u]\}}_{y=1} \right)$$

By just relaxing $y \in \{0,1\}$ to $y \in [0,1]$, one does not get this set.



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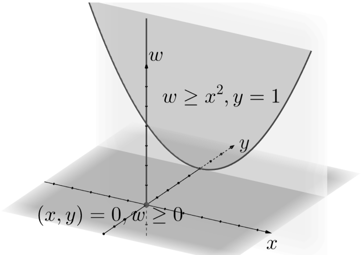
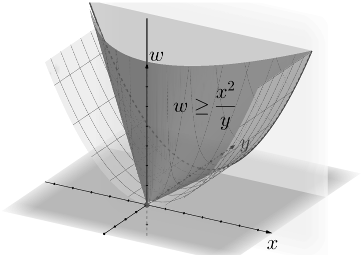
However, replacing $x^2 \leq w$ by the SOC $x^2 \leq wy$ and $w \geq 0$ is sufficient.

[Günlük and Linderoth, 2012]





Convex Hull of Point and Convex Set

More general, consider

$$\{(0,0)\} \quad \cup \quad \{(x,1) \ : \ f(x) \leq 0, \, \ell \leq x \leq u\} \qquad (f \text{ convex})$$

Build the convex combination of both sets:

$$\begin{aligned} \{(x,z) \ : \ & x = \lambda x^1 + (1-\lambda)x^0, \\ & z = \lambda z^1 + (1-\lambda)z^0, \\ & (x^0, z^0) = (0,0), \\ & f(x^1) \leq 0, \ \ell \leq x^1 \leq u, z^1 = 1, \\ & \lambda \in [0,1]\} \end{aligned}$$

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Eliminate fixed variables and substitute $x^1 = x/\lambda$, $z = \lambda$ gives

$$\{(x,y) \; : \; \tilde{f}(x,y) \leq 0, \, \ell y \leq x \leq uy, \; y \in [0,1]\},$$

where $\tilde{f}(x,y) = \begin{cases} y\, f(x/y), & \text{if } y > 0, \\ 0, & \text{if } y = 0, \\ \infty, & \text{otherwise,} \end{cases}$ is the perspective function of $f(x)$.

Important property: If f is convex, then $\tilde{f}$ is convex.

[Günlük and Linderoth, 2012]

Perspective Cuts

Applying the perspective reformulation (replacing $f(x)$ by $\tilde{f}(x, y)$) in a problem can be problematic, because $\tilde{f}(x, y)$ is not differentiable at $y = 0$.

Frangioni and Gentile [2006]: effect of perspective reformulation can be captured in LP relaxation by supporting hyperplanes on the epigraph of $\tilde{f}(x, y)$:

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Frangioni and Gentile [2006]: effect of perspective reformulation can be captured in LP relaxation by supporting hyperplanes on the epigraph of $\tilde{f}(x,y)$:

- linearization of $f(x) \leq 0$ at $x = \hat{x}$:

$$f(\hat{x}) + \nabla f(\hat{x})(x - \hat{x}) \leq 0$$

- perspective cut tilts cut to be tight at $(x,y) = (0,0)$ by adding $(f(0) - f(\hat{x}) + \nabla f(\hat{x})\hat{x})(1-y)$:

$$f(\hat{x})y + \nabla f(\hat{x})(x - \hat{x}y) + f(0)(1-y) \leq 0$$

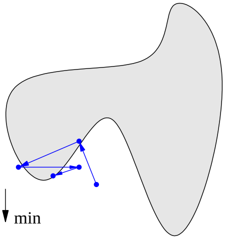
Further Techniques

Primal Side (Find Feasible Solutions)

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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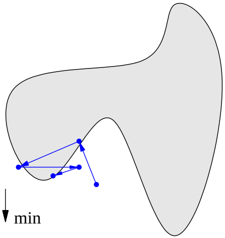

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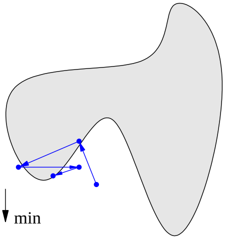

Multistart: run local NLP solver from random starting points to increase likelihood of finding global optimum

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

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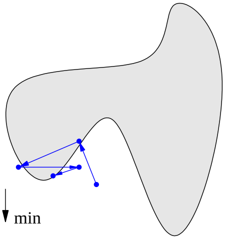

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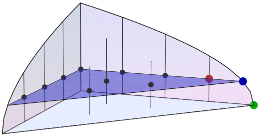
NLP-Diving: solve NLP relaxation, restrict bounds on fractional variable, repeat

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

- Fix nonlinear variables, so problem becomes MIP
- 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



Sub-MIP / Sub-MINLP Heuristics

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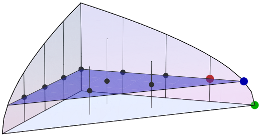
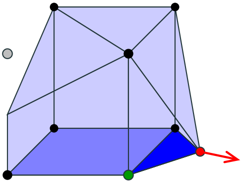


Large Neighborhood Search [Berthold et al., 2011]:

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



Feasibility Pump [D'Ambrosio, Frangioni, Liberti, and Lodi, 2010, 2012, Belotti and Berthold, 2017]:

- originally for MIP [Fischetti, Glover, and Lodi, 2005]
- MINLP: 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)
- Geißler, Morsi, Schewe, and Schmidt [2017]: modifications for convergent algorithm (avoid cycling)

Solver Software

Solvers

The following gives a list of MINLP solvers.

- it is incomplete
- omitted solvers that do not seem to be maintained anymore
- omitted continuous-only (NLP) solvers, e.g., COCONUT [Neumaier, 2001], Ibex (`http://www.ibex-lib.org`), RAPOSa [González-Rodríguez et al., 2022], ...
- omitted solvers without guarantee for global optimality
- solver surveys:
  - Kronqvist, Bernal, Lundell, and Grossmann [2019]
  - Bussieck and Vigerske [2010]

Solver Software

Solvers for Mixed-Integer Quadratic Programs

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CPLEX: https://www.ibm.com/products/ilog-cplex-optimization-studio

- commercial solver by IBM, currently maintenance-only
- available for all modeling languages and APIs to many languages
- convex quadratic objective and constraints
- second-order cone (SOC) constraints
- nonconvex quadratic objective (spatial branch-and-bound)
- branch-and-bound with LP and SOCP (SOC program) relaxation

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MINOTAUR: [Mahajan, Leyffer, Linderoth, Luedtke, and Munson, 2021]
https://github.com/coin-or/minotaur

- open-source solver by IIT Bombay, Argonne Lab, and UW Madison
- available for AMPL and C++ API
- convex and nonconvex quadratic objective and constraints
- spatial branch-and-bound with LP relaxation

Solvers for Mixed-Integer Quadratic Programs (cont.)

MOSEK: https://www.mosek.com

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Pajarito: [Coey, Lubin, and Vielma, 2020] https://github.com/jump-dev/Pajarito.jl

- open-source solver by Chris Coey, Miles Lubin, and Juan Pablo Vielma
- available for JuMP, implemented in Julia
- SOC constraints, and other cones
- outer-approximation algorithm

Solvers for Mixed-Integer Quadratic Programs (cont.)

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- available for JuMP, implemented in Julia
- SOC constraints, and other cones
- outer-approximation algorithm

SMIQP: [Elloumi and Lambert, 2019] https://github.com/amelie-lambert/SMIQP

- open-source solver by Amélie Lambert (CNAM CEDRIC, Paris)
- spatial branch-and-bound with quadratic convex relaxation (constructed via QCR method)

Solver Software

Solvers for Convex MINLP

Solvers for Convex MINLP

AOA: https://documentation.aimms.com/platform/solvers/aoa.html

- integrated in AIMMS modeling system
- outer-approximation algorithm

DICOPT: [Kocis and Grossmann, 1989]

https://distdocs.gams.com/49/docs/S_DICOPT.html

- integrated in GAMS modeling system
- outer-approximation algorithm

Solvers for Convex MINLP

AOA: https://documentation.aimms.com/platform/solvers/aoa.html

- integrated in AIMMS modeling system
- outer-approximation algorithm

DICOPT: [Kocis and Grossmann, 1989]
https://distdocs.gams.com/49/docs/S_DICOPT.html

- integrated in GAMS modeling system
- outer-approximation algorithm

Juniper: [Kröger, Coffrin, Hijazi, and Nagarajan, 2018]
https://github.com/lanl-ansi/juniper.jl

- open-source solver by Los Alamos Lab
- available for JuMP, implemented in Julia
- NLP-based branch-and-bound

Solvers for Convex MINLP (cont.)

Knitro: https://www.artelys.com/solvers/knitro

- commercial solver by Artelys
- available for several modeling systems and many APIs
- LP/NLP-based branch-and-bound, mixed-integer sequential quadratic programming

Solvers for Convex MINLP (cont.)

Knitro: https://www.artelys.com/solvers/knitro

- commercial solver by Artelys
- available for several modeling systems and many APIs
- LP/NLP-based branch-and-bound, mixed-integer sequential quadratic programming

MINOTAUR: [Mahajan, Leyffer, Linderoth, Luedtke, and Munson, 2021]

https://github.com/coin-or/minotaur

- open-source solver by IIT Bombay, Argonne Lab, and UW Madison
- available for AMPL and C++ API
- LP-, QP-, and NLP-based branch-and-bound with fast warmstarts, outer-approximation

Solvers for Convex MINLP (cont.)

Knitro: https://www.artelys.com/solvers/knitro

- commercial solver by Artelys
- available for several modeling systems and many APIs
- LP/NLP-based branch-and-bound, mixed-integer sequential quadratic programming

MINOTAUR: [Mahajan, Leyffer, Linderoth, Luedtke, and Munson, 2021]
https://github.com/coin-or/minotaur

- open-source solver by IIT Bombay, Argonne Lab, and UW Madison
- available for AMPL and C++ API
- LP-, QP-, and NLP-based branch-and-bound with fast warmstarts, outer-approximation

Muriqui: [Melo, Fampa, and Raupp, 2020] https://wendelmelo.net/software

- open-source solver by Wendel Melo, Marcia Fampa, and Fernanda Raupp
- available for AMPL and GAMS and C++ API
- LP/NLP-based branch-and-bound, outer-approximation, various hybrids

Solvers for Convex MINLP (cont.)

Pavito: https://github.com/jump-dev/Pavito.jl

- open-source solver by Chris Coey, Miles Lubin, and Juan P. Vielma
- available for JuMP, implemented in Julia
- LP/NLP-based branch-and-bound, outer-approximation
- sibling of Pajarito [Coey et al., 2020]

Solvers for Convex MINLP (cont.)

Pavito: https://github.com/jump-dev/Pavito.jl

- open-source solver by Chris Coey, Miles Lubin, and Juan P. Vielma
- available for JuMP, implemented in Julia
- LP/NLP-based branch-and-bound, outer-approximation
- sibling of Pajarito [Coey et al., 2020]

SHOT: [Lundell, Kronqvist, and Westerlund, 2022, Lundell and Kronqvist, 2022]
https://shotsolver.dev

- open-source solver by Andreas Lundell and Jan Kronqvist
- available for AMPL and GAMS, Mathematica, C++ API
- LP-based branch-and-bound and outer-approximation with supporting hyperplanes (EHP algorithm)
- can utilize GUROBI for nonconvex quadratics

Solvers for Convex MINLP (cont.)

Pavito: https://github.com/jump-dev/Pavito.jl

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- LP-based branch-and-bound and outer-approximation with supporting hyperplanes (EHP algorithm)
- can utilize GUROBI for nonconvex quadratics

XPRESS-SLP: https://www.fico.com/en/products/fico-xpress-optimization

- commercial solver by FICO
- available for several modeling systems, several APIs
- mixed-integer sequential linear programming (NLP-based branch-and-bound or sequence of MIP approximations)

Solver Software

Solvers for General MINLP

Solvers for General MINLP

Alpine: [Nagarajan, Lu, Yamangil, and Bent, 2016, Nagarajan, Lu, Wang, Bent, and Sundar, 2019] `https://github.com/lanl-ansi/Alpine.jl`

- open-source solver by LANL-ANSI (Los Alamos)
- available for JuMP, implemented in Julia
- at most polynomials
- adaptive, piecewise-linear McCormick convexification scheme

Solvers for General MINLP

Alpine: [Nagarajan, Lu, Yamangil, and Bent, 2016, Nagarajan, Lu, Wang, Bent, and Sundar, 2019] `https://github.com/lanl-ansi/Alpine.jl`

- open-source solver by LANL-ANSI (Los Alamos)
- available for JuMP, implemented in Julia
- at most polynomials
- adaptive, piecewise-linear McCormick convexification scheme

BARON: [Sahinidis, 1996, Tawarmalani and Sahinidis, 2005, Khajavirad and Sahinidis, 2018] `https://minlp.com`

- commercial solver by The Optimization Firm
- available for AIMMS, AMPL, GAMS, JuMP, and more
- spatial branch-and-bound with LP (sometimes also MIP, NLP) relaxation

Solvers for General MINLP

Alpine: [Nagarajan, Lu, Yamangil, and Bent, 2016, Nagarajan, Lu, Wang, Bent, and Sundar, 2019] `https://github.com/lanl-ansi/Alpine.jl`

- open-source solver by LANL-ANSI (Los Alamos)
- available for JuMP, implemented in Julia
- at most polynomials
- adaptive, piecewise-linear McCormick convexification scheme

BARON: [Sahinidis, 1996, Tawarmalani and Sahinidis, 2005, Khajavirad and Sahinidis, 2018] `https://minlp.com`

- commercial solver by The Optimization Firm
- available for AIMMS, AMPL, GAMS, JuMP, and more
- spatial branch-and-bound with LP (sometimes also MIP, NLP) relaxation

EAGO: [Wilhelm and Stuber, 2020] `https://github.com/PSORLab/EAGO.jl`

- open-source solver by Matthew Wilhelm, PSOR Lab at Uni. of Connecticut
- available for JuMP, implemented in Julia
- propagating McCormick relaxations along the factorable structure of each expression (spatial branch-and-bound without auxiliary variables)

Solvers for General MINLP (cont.)

Gurobi: https://www.gurobi.com

- commercial solver by Gurobi
- available for many modeling languages and APIs to many languages
- spatial branch-and-bound with LP or SOCP (SOC program) relaxation

Solvers for General MINLP (cont.)

Gurobi: https://www.gurobi.com

- commercial solver by Gurobi
- available for many modeling languages and APIs to many languages
- spatial branch-and-bound with LP or SOCP (SOC program) relaxation

Hexaly Optimizer: https://www.hexaly.com/

- commercial solver by Hexaly
- available with its own modeling system and APIs for C++, C#, Python, Java
- set-oriented modeling features (variables that are sets or lists of integers)
- spatial branch-and-bound

Solvers for General MINLP (cont.)

Gurobi: https://www.gurobi.com

- commercial solver by Gurobi
- available for many modeling languages and APIs to many languages
- spatial branch-and-bound with LP or SOCP (SOC program) relaxation

Hexaly Optimizer: https://www.hexaly.com/

- commercial solver by Hexaly
- available with its own modeling system and APIs for C++, C#, Python, Java
- set-oriented modeling features (variables that are sets or lists of integers)
- spatial branch-and-bound

Lindo API: [Lin and Schrage, 2009] https://www.lindo.com

- commercial solver by Lindo Systems, Inc.
- available for LINGO and GAMS; APIs for MATLAB, C++, and other
- spatial branch-and-bound with nonlinear relaxations

Solvers for General MINLP (cont.)

MAiNGO: [Bongartz, Najman, Sass, and Mitsos, 2018]

https://git.rwth-aachen.de/avt-svt/public/maingo

- open-source solver by RWTH Aachen, Germany
- C++ and Python APIs
- propagating McCormick relaxations along the factorable structure of each expression (spatial branch-and-bound without auxiliary variables)

Solvers for General MINLP (cont.)

MAiNGO: [Bongartz, Najman, Sass, and Mitsos, 2018]

https://git.rwth-aachen.de/avt-svt/public/maingo

- open-source solver by RWTH Aachen, Germany
- C++ and Python APIs
- propagating McCormick relaxations along the factorable structure of each expression (spatial branch-and-bound without auxiliary variables)

SCIP: [Achterberg, 2009, Bolusani, Besançon, Bestuzheva, Chmiela, Dionísio, Donkiewicz, van Doornmalen, Eifler, Ghannam, Gleixner, Graczyk, Halbig, Hedtke, Hoen, Hojny, van der Hulst, Kamp, Koch, Kofler, Lentz, Manns, Mexi, Mühmer, Pfetsch, Schlösser, Serrano, Shinano, Turner, Vigerske, Weninger, and Xu, 2024, Bestuzheva, Chmiela, Müller, Serrano, Vigerske, and Wegscheider, 2023] https://www.scipopt.org/

- open-source solver by Zuse Institute Berlin, TU Darmstadt, RWTH Aachen, TU Eindhoven, FAU Erlangen, University of Twente, Uni Bayreuth, GAMS, etc
- available for AMPL, GAMS, JuMP, ...; APIs for C, Matlab, Python, ...
- part of a solver for constraint integer programs
- spatial branch-and-bound with linear relaxation

Solvers for General MINLP (cont.)

XPRESS: https://www.fico.com/en/products/fico-xpress-optimization

- commercial solver by FICO
- available for many modeling languages and APIs to many languages
- spatial branch-and-bound with linear relaxation

End.

Thank you for your attention!

Slides at

https://www.gams.com/~svigerske/

Some MINLP reviews:

- Burer and Letchford [2012]
- Belotti, Kirches, Leyffer, Linderoth, Luedtke, and Mahajan [2013]
- Boukouvala, Misener, and Floudas [2016]
- Kılınç and Sahinidis [2017]
- Kronqvist, Bernal, Lundell, and Grossmann [2019]

Some books:

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

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