

# Global Optimization with SCIP 8

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Felipe Serrano, Stefan Vigerske, Fabian Wegscheider**

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September 8th

Introduction

SCIP 7 (and before)

SCIP 8: updated framework

MINLP features in SCIP

Benchmark

## Introduction

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# What is SCIP?



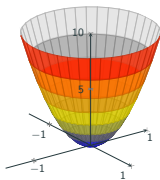
## SCIP (Solving Constraint Integer Programs) ...

- provides a full-scale MIP and MINLP solver,
- incorporates
  - **MIP** features (cutting planes, LP relaxation), and
  - **MINLP** features (spatial branch-and-bound, NLP relaxation)
  - **CP** features (domain propagation),
  - **SAT**-solving features (conflict analysis, restarts),
- is a **branch-cut-and-price** framework,
- has a **modular** structure via plugins,
- is **free for academic** purposes,
- and available in **source-code** under <https://www.scipopt.org>

# Mixed-Integer Nonlinear Programming

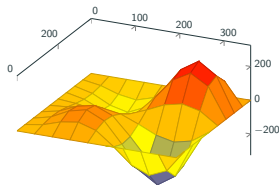
$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & g_k(x) \leq 0 \quad \forall k \in [m] \\ & x_i \in \mathbb{Z} \quad \forall i \in \mathcal{I} \subseteq [n] \\ & x_i \in [\ell_i, u_i] \quad \forall i \in [n] \end{aligned}$$

The functions  $g_k : [\ell, u] \rightarrow \mathbb{R}$  can be



convex

or



nonconvex

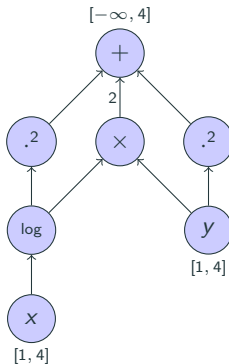
and are given in algebraic form.

# Expression Trees

The **algebraic structure** of nonlinear constraints is stored in a directed acyclic graph:

- nodes: variables, operations
- arcs: flow of computation

$$\log(x)^2 + 2\log(x)y + y^2 \in [-\infty, 4]$$
$$x, y \in [1, 4]$$

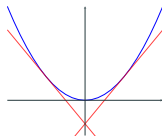


# Branch and Bound

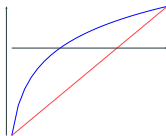
SCIP solves MINLPs by **spatial Branch & Bound**.

**LP relaxation via convexification and linearization:**

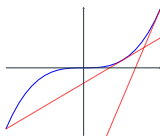
convex functions



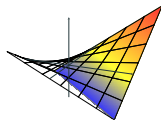
concave functions



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



$x \cdot y$

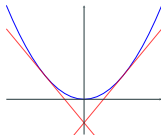


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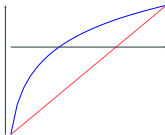
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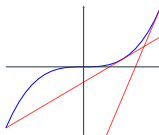
convex functions



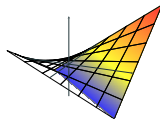
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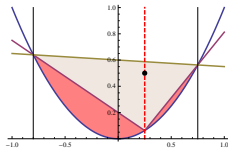
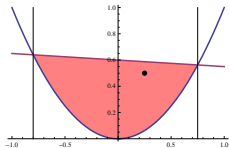
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Branching on variables in violated nonconvex constraints:



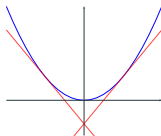


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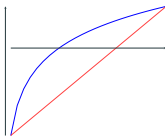
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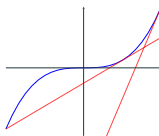
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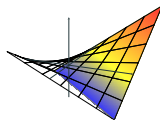
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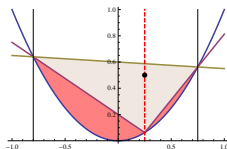
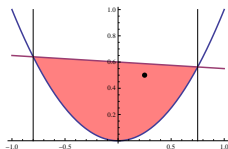
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Branching on variables in violated nonconvex constraints:



... and **bound tightening** (FBBT, OBBT), **primal heuristics** (e.g., sub-NLP/MIP/MINLP), other **special techniques**

## SCIP 7 (and before)

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## Reformulation in Presolve

Goal: Reformulate constraints such that only elementary cases (convex, concave, odd power, quadratic) remain by introducing new variables and new constraints.

Consider

$$\min z$$

$$\text{s.t. } \exp(\ln(1000) + 1 + xy) \leq z$$

$$x^2 + y^2 \leq 2$$

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Reformulation takes apart  $\exp(\ln(1000) + 1 + x y)$ , thus SCIP actually solves the extended formulation

$$\begin{aligned} \min z \\ \text{s.t. } \exp(w) \leq z \\ \ln(1000) + 1 + x y = w \\ x^2 + y^2 \leq 2 \end{aligned}$$

## Issue with explicit reformulation

SCIP solves reformulated problem fine:

```
SCIP Status      : problem is solved [optimal solution found]
Solving Time (sec) : 0.08
Solving Nodes    : 5
Primal Bound     : +9.99999656552062e+02 (3 solutions)
Dual Bound      : +9.99999656552062e+02
Gap              : 0.00 %
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Solution  $(x, y, z, w) = (-1.000574549, 0.999425451, 999.999656552, 6.907754936)$  looks ok:

min z	Violation
s.t. $\exp(w) \leq z$	$0.4659 \cdot 10^{-6} \leq \text{feastol}$ ✓
$\ln(1000) + 1 + xy = w$	$0.6731 \cdot 10^{-6} \leq \text{feastol}$ ✓
$x^2 + y^2 \leq 2$	$0.6602 \cdot 10^{-6} \leq \text{feastol}$ ✓

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However, **original**  $\exp(\ln(1000) + 1 + x y) \leq z$  has **too large violation**:

```
[nonlinear] <e1>: exp((7.9077552789821368151 +1 (<x> * <y>))) -1<z>[C]  <= 0;
violation: right hand side is violated by 0.000673453314561812
best solution is not feasible in original problem
```

## Problem with classic approach

⇒ Explicit reformulation of constraints ...

- ... loses the connection to the original problem.
- ... loses distinction between original and auxiliary variables. Thus, we may branch on auxiliary variables.
- ... prevents simultaneous exploitation of overlapping structures.



## **SCIP 8: updated framework**

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## Avoid explicit split-up of constraints.

- introduce **extended formulation** as **annotation to the original** formulation
- use extended formulation for **relaxation**
- use original formulation for **feasibility checking**
- to resolve infeasibility in original constraints, tighten relaxation of extended formulation

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## Everything nonlinear is an expression.

- represent all nonlinear constraints in **one expression graph** (DAG)
- all algorithms (check, separation, propagation, etc.) work on the same expression graph, no more specialized nonlinear constraints
- **separate expression operators** ( $+$ ,  $\times$ ) and **high-level structures** (quadratic, semi-continuous, second order cone, etc.)

# Expression Handlers

Each **operator type** (+, ×, pow, etc.) is implemented by an **expression handler**, which can provide a number of callbacks:

- **evaluate and differentiate** expression w.r.t. operands
- interval evaluation and **tighten bounds** on operands
- provide linear **under- and over-estimators**
- inform about curvature, monotonicity, integrality
- simplify, compare, print, parse, hash, copy, etc.

Expression handlers are like other **SCIP plugins**.

New ones can be added by users (YOU!).

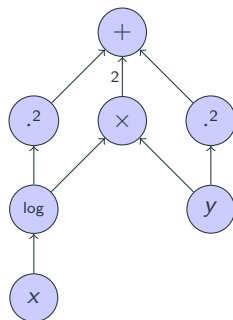
**Available handler:** abs, cos, entropy, exp, log, pow, product, signpow, sin, sum, value, var

## Example: Extended Formulation (exprhdlr only)

**Constraint:**

$$\log(x)^2 + 2 \log(x)y + y^2 \leq 4$$

This formulation is used to **check feasibility** and **presolve**.



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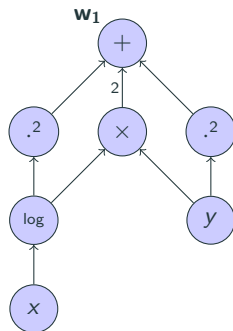
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**Extended Formulation:**

$$w_1 \leq 4$$
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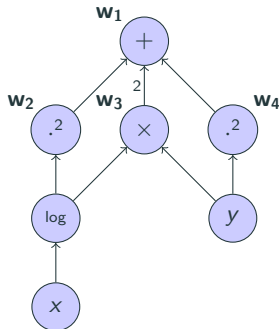
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$$\begin{aligned}w_1 &\leq 4 \\w_2 + 2w_3 + w_4 &= w_1 \\ \log(x)^2 &= w_2 \\ \log(x)y &= w_3 \\ y^2 &= w_4\end{aligned}$$





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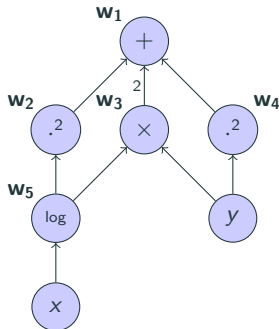
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**Extended Formulation:**

$$\begin{aligned}w_1 &\leq 4 \\w_2 + 2w_3 + w_4 &= w_1 \\w_5^2 &= w_2 \\w_5 y &= w_3 \\y^2 &= w_4 \\\log(x) &= w_5\end{aligned}$$

Used to **construct LP relaxation**.



But  $\log(x)^2 + 2\log(x)y + y^2 \leq 4$  is **convex** and **quadratic** in  $(\log(x), y)$ .

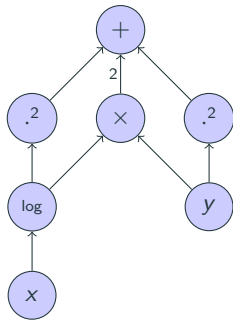
But  $\log(x)^2 + 2\log(x)y + y^2 \leq 4$  is **convex** and **quadratic** in  $(\log(x), y)$ .

To **explore structure**, we now have **Nonlinearity Handler**:

- Adds **additional separation and/or propagation** algorithms for structures that can be identified in the expression graph.
- **Attached to nodes in expression graph**, but **does not define expressions** nor constraints.
- Examples: quadratics, convex and concave, second order cone, . . .
- **Several** nlhdlrs can be attached to a node in the expression graph.

## Example: Extended Formulation (with nlhdlrs)

**Constraint:**  $\log(x)^2 + 2 \log(x)y + y^2 \leq 4$

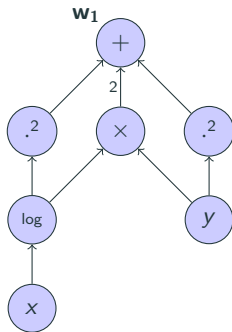


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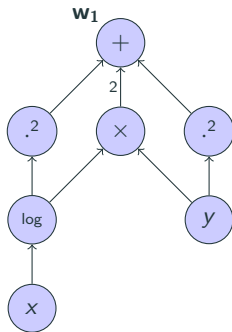


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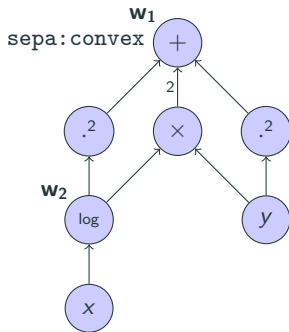
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    - detects a **convex quadratic structure**,
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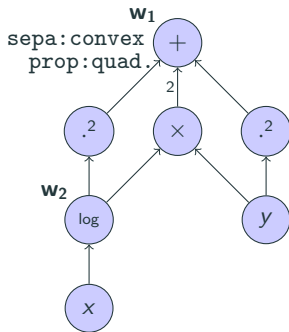
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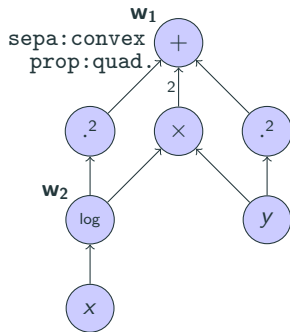
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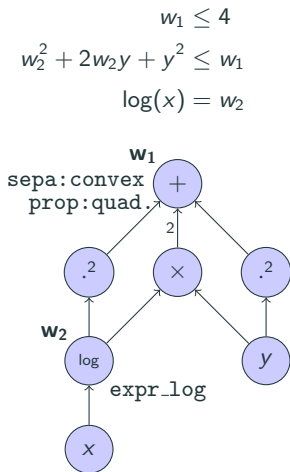
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    - also detects a **quadratic structure**,
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    - **notifies that it will use bounds** of nodes log and y.
3. Run detect of all nlhdlrs on log node.
  - No specialized nlhdlr signals success.  
The **expression handler** will be used for both under/overestimation and propagation.



## MINLP features in SCIP (teasers only)

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SCIP features **particular for nonlinear** structures

**+** = **new** or improved in SCIP 8

- **simplify** expressions
- + identify **common subexpressions**

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- if QP, add **KKT** as redundant constraints
- + **symmetry detection** using expression graph [Liberti 2010, Wegscheider 2019]



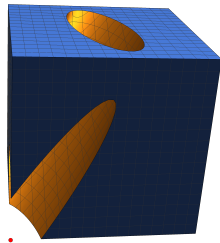
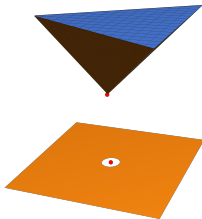
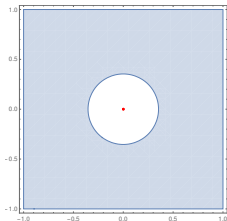
# Quadratics

## Nonlinear handler for quadratic subexpressions:

- provides **domain propagation** (variable bound tightening)

+ **intersection cuts** for nonconvex quadratics

[Chmiela, Muñoz, Serrano 2021]



+ also as separator for implied quadratics  $\det(2 \times 2 \text{ minors of } X) = 0$ ,  $X = xx^T$

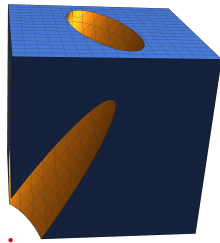
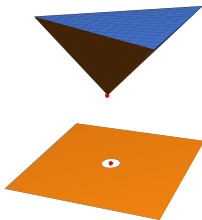
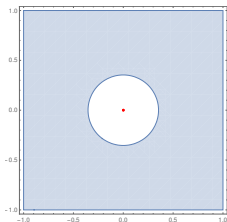
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## Separator for implied PSD constraint ( $X \succeq xx^T$ ):

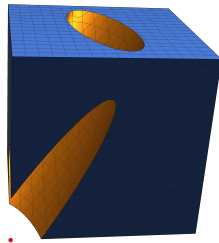
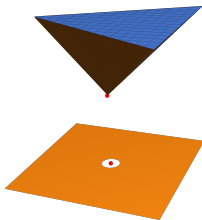
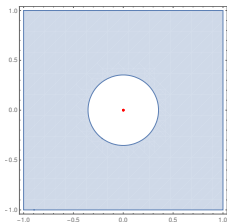
+ SDP-cuts for  $2 \times 2$  principal minors of  $X - xx^T \succeq 0$

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- + **intersection cuts** for nonconvex quadratics

[Chmiela, Muñoz, Serrano 2021]



- + also as separator for implied quadratics  $\det(2 \times 2 \text{ minors of } X) = 0$ ,  $X = xx^T$

## Separator for implied PSD constraint ( $X \succeq xx^T$ ):

- + SDP-cuts for  $2 \times 2$  principal minors of  $X - xx^T \succeq 0$

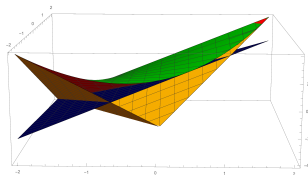
## Separator for edge-concave quadratics:

- **aggregate** quadratic constraints to be edge-concave
- **separate facets** from vertex-polyhedral convex hull

[Misener, Floudas 2012]

## Nonlinear handler for bilinear expressions:

- convexify and domain propagation for  $xy$  w.r.t. **additional inequalities** on  $x$ ,  $y$ , e.g.,  $x \leq y$

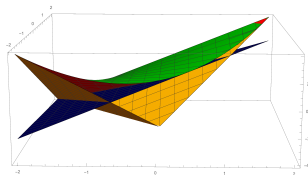


- inequalities found by 2D-projection of LP relaxation ( $\approx$  OBBT)

[Linderoth 2004, Hijazi 2015, Locatelli 2016, Müller, Serrano, Gleixner 2020]

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[Linderoth 2004, Hijazi 2015, Locatelli 2016, Müller, Serrano, Gleixner 2020]

## Reformulation Linearization Technique for bilinear products:

- + cuts from multiplication of LP rows and bounds
- + also for **implicit products** in mixed-binary linear problems

[Adams, Sherali 1986, Achterberg, Bestuzheva, Gleixner 2022+]

# Second-Order Cones

Nonlinear handler for Second-Order Cones:

- + **detect** SOC constraints from quadratics and some Euclidean norms



# Second-Order Cones

## Nonlinear handler for Second-Order Cones:

- + **detect** SOC constraints from quadratics and some Euclidean norms
- separate using **disaggregated formulation**

[Vielma, et.al. 2016]

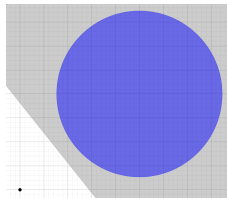


# Convexity and Concavity

## Nonlinear handler for convex and concave expressions:

- + find convex/concave subexpressions using composition rules
  - gradient cuts on convex functions
  - facets of convex hull on concave function
- + prefer extended formulations for convex case

[Tawarmalani Sahinidis, 2005]



[Veinott 1967, Kronqvist, Lundell, Westerlund 2016, Serrano, Schwarz, Gleixner 2020]

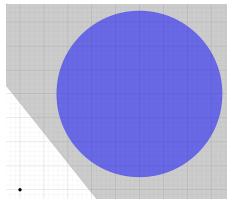


# Convexity and Concavity

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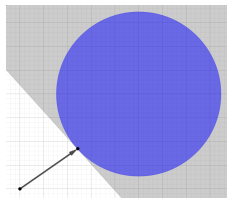
- + find convex/concave subexpressions using composition rules
  - gradient cuts on convex functions
  - facets of convex hull on concave function
- + prefer extended formulations for convex case

[Tawarmalani Sahinidis, 2005]



## Separator for supporting hyperplanes:

- separators to linearize at **boundary of convex** NLP relaxation
- **projection** of given point, or **linesearch** to interior point



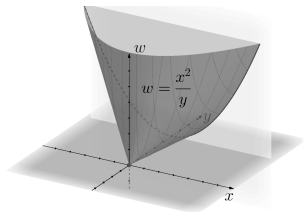
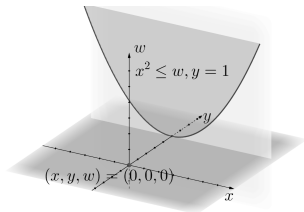
[Veinott 1967, Kronqvist, Lundell, Westerlund 2016, Serrano, Schwarz, Gleixner 2020]

# Perspective Strengthening

Nonlinear handler for perspective strengthening:

- + detect expressions in semi-continuous variables ( $\ell_x y \leq x \leq u_x y$ ,  $y \in \{0, 1\}$ )
- + strengthen under/overestimators for such expressions, e.g.,

$$f(\hat{x}) + \nabla f(\hat{x})(x - \hat{x}) \leq w \quad \Rightarrow \quad f(\hat{x})y + \nabla f(\hat{x})(x - \hat{x}y) \leq w$$



[Frangioni, Gentile 2006, Bestuzheva, Gleixner, Vigerske 2021]

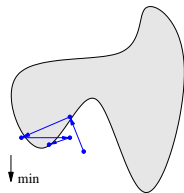
## Nonlinear handler for quotients:

- to avoid ambiguity, there is no expression type for quotients
- + detect  $\frac{ax+b}{cy+d}$  in nonlinear handler
- + provide bound tightening
- + provide linear under/overestimates

[Zamora, Grossmann 1998]

# Primal Heuristics

- fix all integer vars, **solve NLP** to local optimality



- multistart** with constraint consensus for NLPs

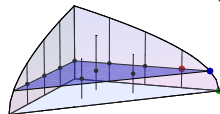
[Smith, Chinneck, Aitken 2013]

- NLP-diving**

- solve sequence of **regularized NLP reformulations** of MINLP (“MPEC”)

- fix nonlinear vars, **solve remaining sub-MIP**

[Berthold, Gleixner 2014]



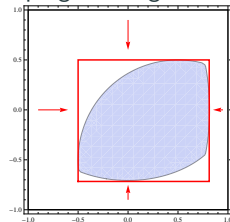
- other **large neighborhood search** heuristics, solving sub-MINLPs

[Berthold, Heinz, Pfetsch, Vigerske 2011]

NLP solving via Ipopt and CppAD

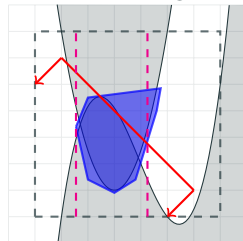
# Domain Propagation (Variable Bound Tightening)

- Feasibility-Based Bound Tightening (FBBT): as in constraint programming



- Optimization-Based Bound Tightening (OBBT): optimize var. over LP

[Gleixner, Berthold, Müller, Weltge 2017]



- OBBT over NLP relaxation

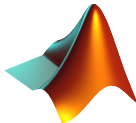
# Interfaces

Readers for MINLP included:

- MPS, LP, PIP, AMPL NL, OSiL, ZIMPL

Interfaces:

- C, Java
- Python
- Julia, Matlab
- AMPL, GAMS
- ...



## Benchmark

---

# Benchmark Setting

## Test set:

- 183 “solvable” instances from MINLPLib
- varying degree of integrality
- varying degree of nonlinearity
- avoid too many instances with similar name
- all solvers can handle (no sine, cosine, signpower)



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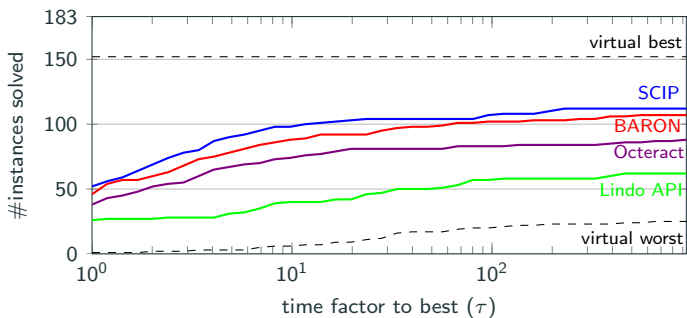
## Settings:

- relative gap tolerance  $10^{-4}$
- feasibility tolerance  $10^{-6}$
- bound unbounded variables by  $10^{12}$
- 2 hours time limit
- 1 thread
- 50 GB RAM

**GAMS:** all included global (still updated) MINLP solvers

## Comparison

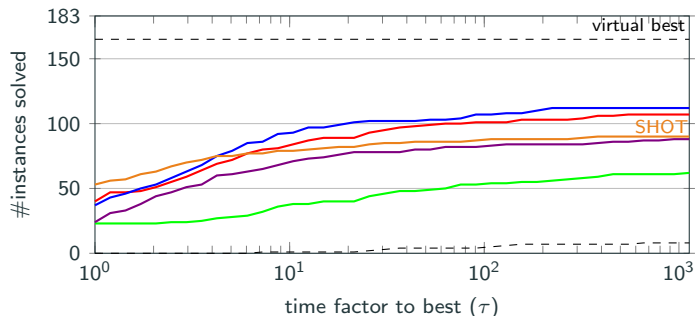
	solved	timeout	mean time*
BARON 22.9.1	107	72	616s
Lindo API 13.0.340	62	80	1116s
Octeract 4.4.1	88	85	849s
SCIP 8.0 (f0a1490e3b)	112	66	497s
virtual best	152	–	109s



\*w.r.t. 135 instances on which no solver returned wrong results

## Comparison incl. SHOT with Gurobi

	solved	timeout	mean time <sup>†</sup>
BARON 22.9.1	107	72	627s
Lindo API 13.0.340	62	80	1155s
Octeract 4.4.1	88	85	824s
SCIP 8.0 (f0a1490e3b)	112	66	470s
SHOT 1.1 (033622c6) with Gurobi 9.5.2	90	18	(59s)
virtual best	165	–	(29s)



<sup>†</sup> w.r.t. 129 instances on which no solver returned wrong results

# End!

For details, see also the [release report](#) of SCIP 8 (and previous, and reference therein):

K. Bestuzheva, M. Besançon, W. Chen, A. Chmiela, T. Donkiewicz, J. Doornmalen, L. Eifler, O. Gaul, G. Gamrath, A. Gleixner, L. Gottwald, C. Graczyk, K. Halbig, A. Hoen, C. Hojny, R. Hulst, T. Koch, M. Lübbecke, S. Maher, F. Matter, E. Mühmer, B. Müller, M. Pfetsch, D. Rehfeldt, S. Schlein, F. Schlösser, F. Serrano, Y. Shinano, B. Sofranac, M. Turner, S. Vigerske, F. Wegscheider, P. Wellner, D. Weninger, J. Witzig, *The SCIP Optimization Suite 8.0*, ZIB Report 21-41, 2021

## PS: Testset

arki0005 arki0019 arki0020 autocorr\_bern25-13 autocorr\_bern30-04 autocorr\_bern35-04 ball\_mk4\_15  
batchs201210m bayes2\_20 bayes2\_30 bayes2\_50 blend146 blend480 blend852 camshape100 camshape200  
cardqp\_inlp cardqp\_iqp carton9 casctanks cecil\_13 celar6-sub0 cesam2log chimera\_k64maxcut-01  
chimera\_k64maxcut-02 chimera\_lga-01 chp\_shorttermplan1a chp\_shorttermplan2a chp\_shorttermplan2b  
clay0305hfsg color\_lab3\_3x0 crossdock\_15x7 crossdock\_15x8 crudeoil\_pooling-ct3 crudeoil\_pooling-dt2  
crudeoil\_pooling-dt4 cvxnonsep\_psig20 cvxnonsep\_psig30 edgexcross10-050 edgexcross10-070 edgexcross14-039  
eg\_all\_s eigena2 elec25 ex1223b ex1233 ex1252 ex4 ex5\_3\_3 ex5\_4\_4 ex6\_1\_3 ex6\_2\_10 ex6\_2\_6 ex7\_2\_3  
ex8\_5\_2 ex8\_5\_6 faclay20h flay05h flay05m flay06m fo7\_2 fo7\_ar2\_1 fo7\_ar3\_1 gabriel01 gabriel02 gabriel04  
gastrans135 gastrans582\_cold13 gastrans582\_cold17\_95 graphpart\_3pm-0444-0444 graphpart\_clique-30  
graphpart\_clique-40 gsg\_0001 hadamard\_5 heatexch\_spec2 ibs2 ising2\_5-300.5555 kall\_circles\_c8a  
kall\_congruentcircles\_c61 kall\_diffcircles\_9 kissing2 kport20 kriging\_peaks-red020 kriging\_peaks-red030  
kriging\_peaks-red050 lop97ic maxcsp-geo50-20-d4-75-36 maxcsp-langford-3-11 meanvar-orl400\_05\_e\_7  
methanol100 methanol200 milinfract multiplants\_mtg2 multiplants\_mtg5 multiplants\_stg6  
nd\_netgen-2000-2-5-a-a-ns\_7 nd\_netgen-3000-1-1-b-b-ns\_7 netmod\_dol1 netmod\_dol2 nous1 nvs04 nvs05  
nvs06 orth\_d3m6 parabol5\_2\_3 parallel p\_ball\_10b\_5p\_2d\_h p\_ball\_20b\_5p\_3d\_m p\_ball\_30b\_5p\_2d\_m  
pedigree\_ex1058 pedigree\_ex485 pedigree\_sp\_top4\_350tr pinene100 pinene200 pinene50 pointpack08  
pointpack10 pooling\_digabel16 pooling\_epa1 pooling\_epa2 popdynm100 popdynm25 popdynm50  
portfol\_robust100\_09 portfol\_robust200\_03 portfol\_shortfall100\_04 powerflow0009r powerflow0030r  
qspp\_0\_10\_0\_1\_10\_1 qspp\_0\_13\_0\_1\_10\_1 qspp\_0\_14\_0\_1\_10\_1 radar-2000-10-a-6\_lat\_7 radar-3000-10-a-8\_lat\_7  
rocket100 rocket200 rocket50 rsyn0820m03m rsyn0820m04m rsyn0840m04m sepasequ\_convent  
sfacloc2\_2\_80 sfacloc2\_3\_90 sfacloc2\_4\_90 sjup2 sonet19v5 sonet20v6 sonet24v2 sonetgr17  
sporttournament22 sporttournament26 sporttournament28 sqfl020-150 sqfl030-150 sqfl030-150persp  
sssd15-06persp sssd15-08 sssd15-08persp st\_e32 st\_e36 steenbrf supplychainp1\_022020  
supplychainr1\_022020 syn40m04hfsg synheat telecomsp\_pacbell tln7 tls4 toroidal3g7\_6666 tspn10 tspn12  
unitcommit\_200\_100\_1\_mod\_8 unitcommit\_200\_100\_2\_mod\_8 unitcommit\_50\_20\_2\_mod\_8 wastepaper3  
wastepaper4 wastewater05m2 wastewater13m2 wastewater14m1 waterno2\_03 waterno2\_04 waterund11  
waterund14 waterund22