Revising the handling of nonlinear constraints in SCIP

Work in Progress Report

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SCIP: Solving Constraint Integer Programs

- modular branch-cut-and-price framework for constraint integer programming
- includes full-fledged MIP/MINLP solver
- part of SCIP Optimization Suite (GCG, SCIP, SoPlex, UG, ZIMPL)
- Latest Release Report: The SCIP Optimization Suite 6.0 by Gleixner, Bastubbe, Eifler, Gally, Gamrath, Gottwald, Hendel, Hojny, Koch, Lübbecke, Maher, Miltenberger, Müller, Pfetsch, Puchert, Rehfeldt, Schlösser, Schubert, Serrano, Shinano, Viernickel, Wegscheider, Witt, Witzig

Download at scip.zib.de: SCIP Optimization Suite SCIP SoPlex ZIMPL UG GCG SCIP Solving Constraint Integer Programs About About SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access License How To Cite Platforms Developers Workshop Related Work Exact MIP PolySCIP

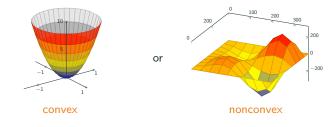
By default, SCIP comes with a bouquet of different plugins for solving MIPs and MINLPs.

• free for academic use

Mixed-Integer Nonlinear Programming

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

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

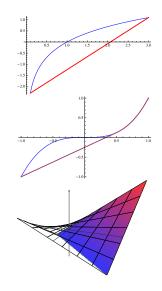


and are given in algebraic form.

SCIP solves MINLPs by spatial Branch & Bound

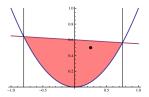
Ingredients:

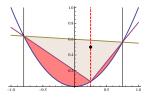
- constructing an LP relaxation by
 - relaxing integrality
 - convexifying non-convexities



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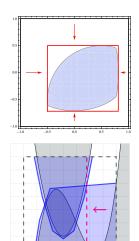
- constructing an LP relaxation by
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- branching on
 - fractional integer variables
 - variables in violated nonconvex constraints





Ingredients:

- constructing an LP relaxation by
 - relaxing integrality
 - convexifying non-convexities
- branching on
 - fractional integer variables
 - · variables in violated nonconvex constraints
- tightening of variable bounds (domain propagation)
- primal heuristics
- presolving / reformulation



Current Implementation (SCIP 6.0)

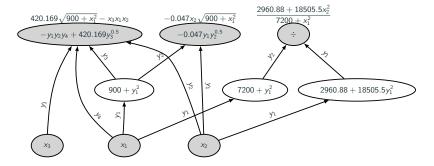
Expression trees and graphs

cons_nonlinear (lhs $\leq \sum_{i=1}^{n} a_i x_i + \sum_{j=1}^{m} c_j f_j(x) \leq rhs$) stores the nonlinear functions f_j of

all constraints in one expression graph (DAG).

For example (MINLPLib instance nvs01):

$$\begin{split} 420.169 \sqrt{900+x_1^2} - x_3 x_1 x_2 = 0 \qquad & \frac{2960.88 + 296088 \cdot 0.0625 x_2^2}{7200+x_1^2} - x_3 \geq 0 \\ & x_{obj} - 0.047 x_2 \sqrt{900+x_1^2} \geq 0 \end{split}$$



• some use of common subexpression

Expression operators and constraint handler

Operators (handled by cons_nonlinear):

- variable index, constant
- +, -, *, ÷
- \cdot^2 , $\sqrt{\cdot}$, \cdot^p $(p \in \mathbb{R})$, \cdot^n $(n \in \mathbb{Z})$, $x \mapsto x |x|^{p-1}$ (p > 1)
- exp, log
- min, max, abs
- \sum , \prod , affine-linear, quadratic, signomial
- (user)

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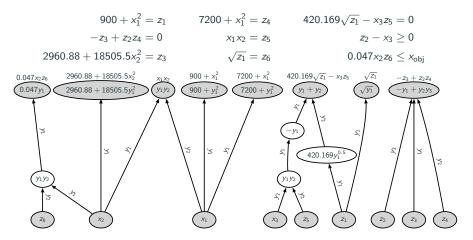
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Additional constraint handler:

- quadratic
- abspower $(x \rightarrow x |x|^{p-1}, p > 1)$
- SOC (second-order cones)
- (bivariate)

Reformulation in cons_nonlinear (during presolve)

Goal: Reformulate constraints such that only elementary cases (convex, concave, odd power, quadratic) remain.



- reformulates constraints by introducing new variables and new constraints
- other constraint handler can participate

Problem with this approach

An optimal solution: min z x = -1s.t. $\exp(\ln(1000) + 1 + xy) \le z$ y = 1

z = 1000

Consider

 $x^2 + y^2 \le 2$

Problem with this approach

z

An optimal solution:

Consider	min z s.t. $\exp(\ln(1000) + 1 + xy) \le z$ $x^2 + y^2 \le 2$	x = -1 y = 1 z = 1000
SCIP reports		
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 % [nonlinear] <e1>: exp((7.9077552789821368151 +1 (<x> * <y>)))-1<z>[C] <= 0;</z></y></x></e1>		
x y	-1.00057454873626 0.999425451364613	(obj:0) (obj:0)

999.999656552061 (obj:1)

Reformulated problem

Reformulation takes apart exp(ln(1000) + 1 + xy), thus SCIP actually solves

min z
s.t.
$$\exp(w) \le z$$

 $\ln(1000) + 1 + xy = w$
 $x^2 + y^2 \le 2$

min z

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Violation $0.4659 \cdot 10^{-6} \le \text{numerics/feastol } \checkmark$ $0.6731 \cdot 10^{-6} \le \text{numerics/feastol } \checkmark$ $0.6602 \cdot 10^{-6} \le \text{numerics/feastol } \checkmark$

Solution (found by <relaxation>):

 $\begin{array}{rrrr} x = & -1.000574549 \\ y = & 0.999425451 \\ z = 999.999656552 \\ w = & 6.907754936 \end{array}$

min z

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 - ... looses the connection to the original problem.

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- \Rightarrow Explicit reformulation of constraints ...
 - ... looses the connection to the original problem.
 - ... looses distinction between original and auxiliary variables. Thus, we may branch on auxiliary variables.
 - ... prevents simultaneous exploitation of overlapping structures.

A new framework for NLP in SCIP (work in progress)

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Fundamental structure

Everything is an expression.

- ONE constraint handler: cons_expr
- represent all nonlinear constraints in one expression graph (DAG)

 $\mathsf{lhs} \leq \mathsf{expression}\mathsf{-node} \leq \mathsf{rhs}$

• all algorithms (check, separation, propagation, etc.) work on the expression graph (no upgrades to specialized nonlinear constraints)

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- separate expression operators $(+, \times)$ and high-level structures (quadratic, etc.)
- \Rightarrow avoid redundancy / ambiguity of expression types (classic: +, \sum , linear, quad., ...)
 - stronger identification of common subexpressions

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Do not reformulate constraints.

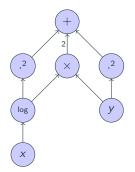
• introduce auxiliary variables for the relaxation only

Constraint:

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

This formulation is used to

- check feasibility,
- presolve,
- propagate domains, ...



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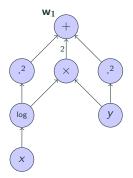
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(Implicit) Reformulation:

$$w_1 \le 4$$

 $\log(x)^2 + 2\log(x)y + y^2 = w_1$



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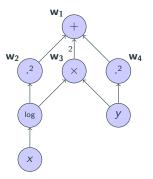
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(Implicit) Reformulation:

$$w_1 \le 4$$

 $w_2 + 2w_3 + w_4 = w_1$
 $\log(x)^2 = w_2$
 $\log(x)y = w_3$
 $y^2 = w_4$



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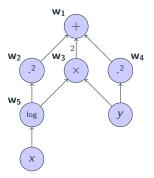
$$w_2 + 2w_3 + w_4 = w_1$$

$$w_5^2 = w_2$$

$$w_5y = w_3$$

$$y^2 = w_4$$

$$\log(x) = w_5$$



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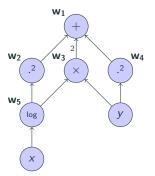
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$$\log(x) = w_5$$



Used to construct LP relaxation.

Each operator type $(+, \times, pow, etc.)$ 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
- distribute branching scores to operands
- inform about curvature, monotonicity, integrality
- simplify, compare, print, parse, hash, copy, etc.

Expression handler are like other SCIP plugins, thus new ones can be added by users.

```
min z s.t. \exp(\ln(1000) + 1 + xy) \le z, x^2 + y^2 \le 2
```

Classic:

```
presolving (5 rounds: 5 fast, 1 medium, 1 exhaustive):
0 deleted vars, 0 deleted constraints, 1 added constraints,...
0 implications, 0 cliques
presolved problem has 4 variables (0 bin, 0 int, 0 impl, 4 cont)
and 3 constraints
2 constraints of type <quadratic>
1 constraints of type <quadratic>
```

[...]

```
      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 %

      [nollinear] <el>: exp((7.90776 + (<x > <y>)))-1<<z>[C] <= 0;</td>

      violation: right hand side is violated by 0.000673453314561812

      best solution is not feesible in original problem
```

x	-1.00057454873626	(obj:0)
У	0.999425451364613	(obj:0)
z	999.999656552061	(obj:1)

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min z s.t. \exp(\ln(1000) + 1 + xy) \le z, x^2 + y^2 \le 2
```

Classic:

New:

```
presolving (5 rounds: 5 fast, 1 medium, 1 exhaustive): presolving (3 rounds: 3 fast, 1 medium, 1 exhaustive):
0 deleted vars, 0 deleted constraints, 1 added constraints,... 0 deleted vars, 0 deleted constraints, 0 added constraints,... 0 implications, 0 cliques
presolved problem has 4 variables (0 bin, 0 int, 0 impl, 4 cont) presolved problem has 3 variables (0 bin, 0 int, 0 impl, 3 cont)
and 3 constraints of type <quadratic> 2 constraints of type <quadratic> 2 constraints of type <constraints of type <constraints of type <constraints of type <constraints</pre>
```

[...]

[...]

	SCIP Status	:	problem is solved [optimal solution found]	SCIP Status	: problem is solved [optimal solution found]
	Solving Time (sec)	:	0.08	Solving Time (sec)	: 0.47
	Solving Nodes	:	5	Solving Nodes	: 15
	Primal Bound	:	+9.99999656552062e+02 (3 solutions)	Primal Bound	: +9.99999949950021e+02 (2 solutions)
	Dual Bound	:	+9.99999656552062e+02	Dual Bound	: +9.99999949950021e+02
	Gap	:	0.00 %	Gap	: 0.00 %
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- -1.0000002499999 (obj:0)
- 1.0000002499999 (obj:0)
- 999.999949950021 (obj:1)

Performance

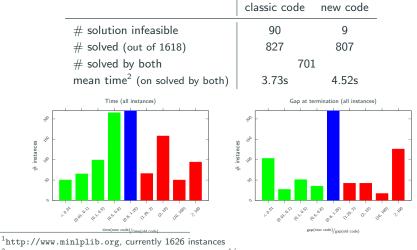
- Testset: 1618 instances from MINLPLib¹
- Time limit: 30 minutes, Optimality gap tolerance: 0.01%
- LP solver: CPLEX 12.9.0.0, NLP solver: IPOPT 3.12.11

	classic code	new code
# solution infeasible	90	9

¹http://www.minlplib.org, currently 1626 instances ²shifted geometric mean with shift = 1s: $\prod_{i=1}^{n} (t_i + 1)^{1/n} - 1$

Performance

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A new framework for NLP in SCIP (work in progress)

Acceleration

Exploiting structure

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

Smarter reformulation:

• Recognize that $\log(x)^2 + 2\log(x)y + y^2$ is convex in $(\log(x), y)$.

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- \Rightarrow Introduce auxiliary variable for log(x) only.

$$w^2 + 2wy + y^2 \le 4$$
$$\log(x) = w$$

Handle $w^2 + 2wy + y^2 \le 4$ as convex constraint ("gradient-cuts").

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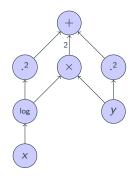
Handle $w^2 + 2wy + y^2 \le 4$ as convex constraint ("gradient-cuts").

Nonlinearity Handler:

- Adds additional separation and propagation algorithms for structures that can be identified in the expression graph.
- Attached to nodes in expression graph, but does not *define* expressions or constraints.
- Examples: quadratics, convex subexpressions, vertex-polyhedral

- Nodes in the expression graph can have one or several nlhdlrs attached.
- At beginning of solve, detection callbacks are run **only** for nodes that have auxiliary variable. Detection callback may add auxiliary variables.

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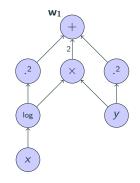


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$$w_1 \leq 4$$

1. Add auxiliary variable w_1 for root.

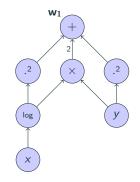


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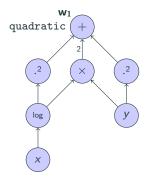


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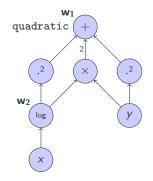


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 $w_2^2 + 2w_2y + y^2 \leq w_1 \quad [nlhdlr_quadratic]$

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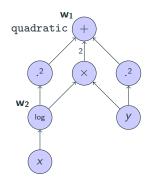


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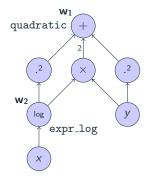


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$$w_1 \leq 4$$

 $w_2^2 + 2w_2y + y^2 \leq w_1 \quad [nlhdlr_quadratic]$
 $\log(x) = w_2 \quad [expr_log]$

- 1. Add auxiliary variable w_1 for root.
- 2. Run detect of all nlhdlrs on + node.
 - nlhdlr_quadratic detects a convex quadratic structure and signals success.
 - nlhdlr_quadratic adds an auxiliary variable w₂ for log node.
- 3. Run detect of all nlhdlrs on log node.
 - No specialized nlhdlr signals success. The expression handler will be used.

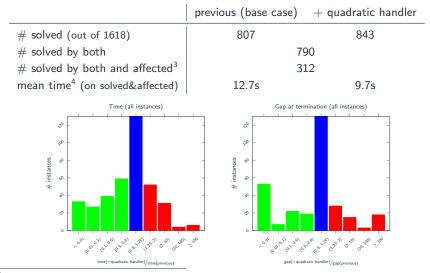


- Recognize quadratic forms (sums of squares and products in two terms).
- Recognize convexity by checking coefficient matrix for positive semidefiniteness. Use this to provide tight linear underestimators by linearization.
- Provide better bound tightening, in particular for univariate quadratics:

$$\{ax^{2} + bx : x \in [\ell, u]\} = \begin{cases} \operatorname{conv}\{a\ell^{2} + b\ell, au^{2} + bu, -\frac{b^{2}}{4a}\}, & \text{if } -\frac{b}{2a} \in [\ell, u], \\ \operatorname{conv}\{a\ell^{2} + b\ell, au^{2} + bu\}, & \text{otherwise} \end{cases}$$

$$\{x : ax^{2} + bx \ge c\} = \begin{cases} \left[-\infty, -\sqrt{\frac{c}{a} + \frac{b^{2}}{4a^{2}}} - \frac{b}{2a}\right] \cup \left[\sqrt{\frac{c}{a} + \frac{b^{2}}{4a^{2}}} - \frac{b}{2a}, \infty\right], & \text{if } a > 0, \\ -\sqrt{\frac{c}{a} + \frac{b^{2}}{4a^{2}}} - \frac{b}{2a}, \sqrt{\frac{c}{a} + \frac{b^{2}}{4a^{2}}} - \frac{b}{2a}} \end{cases}, & \text{if } a < 0. \end{cases}$$

Impact of handler for quadratics



³affected = different search path, indicated by different number of B&B nodes or LP iterations ⁴shifted geometric mean with shift = 1s: $\prod_{i=1}^{n} (t_i + 1)^{1/n} - 1$

Separator for RLT

- for bilinear products $x_i x_j$, we may have introduced auxiliary variables $w_{i,j}$
- the expression handler for products generates McCormick inequalities:

$$\begin{aligned} &(x_i - \ell_i)(x_j - \ell_j) \ge 0 & \Rightarrow & w_{i,j} \ge \ell_i x_j + \ell_j x_i - \ell_i \ell_j \\ &(x_i - u_i)(x_j - u_j) \ge 0 & \Rightarrow & w_{i,j} \ge u_i x_j + u_j x_i - u_i u_j \\ &(x_i - \ell_i)(x_j - u_j) \le 0 & \Rightarrow & w_{i,j} \le \ell_i x_j + u_j x_i - \ell_i u_j \\ &(x_i - u_i)(x_j - \ell_j) \le 0 & \Rightarrow & w_{i,j} \le u_i x_j + \ell_j x_i - u_i \ell_j \end{aligned}$$



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Reformulation-Linearization Technique [Adams and Sherali, 1986]:

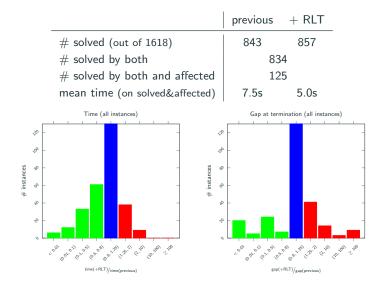
• additional valid cuts can be obtained by multiplication with linear constraints:

$$a^{\mathsf{T}} x \ge b \quad \times \quad x_j - \ell_j \qquad \Rightarrow \quad a^{\mathsf{T}} w_{\cdot,j} - a^{\mathsf{T}} x \, \ell_j \ge b x_j - b \, \ell_j$$

$$a^{\mathsf{T}} x = b \quad \times \quad x_j \qquad \Rightarrow \quad a^{\mathsf{T}} w_{\cdot,j} = b x_j$$

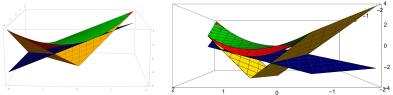
- in our implementation, we only look for RLT cuts that do not introduce new auxiliary variables *w*_{*i*,*j*}
- very effective for pooling problems

Impact of RLT separator



Tighter convex relaxations for bilinear terms

- McCormick inequalities give convex hull for $x_i x_j$ on box $[\ell_i, \ell_j] \times [u_i, u_j]$
- they do not if additional inequalities are present, e.g., $x_i \leq x_j$:



green — graph of $w_{ij} = x_i x_j$

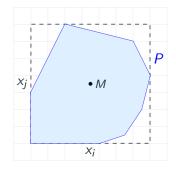
yellow — McCormick relaxation of $x_i x_j$ over $[-2, 2]^2$

red — convex envelope of $x_i x_j$ over $\{(x_i, x_j) \in [-2, 2]^2 : x_i \leq x_j\}$

closed formulas and algorithms are known [Linderoth 2004, Hijazi 2015, Locatelli 2016]

Problem: inequalities utilizing only x_i and x_j may not be present in problem **Solution**⁵: Project LP relaxation onto (x_i, x_j) , $P := \text{proj}_{x_i, x_i}(\text{LP})$

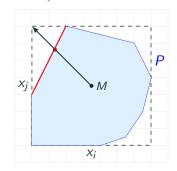
- assume variable bounds are tight
- $M := \left(\frac{u_i + \ell_i}{2}, \frac{u_j + \ell_j}{2}\right) \in P$
- every facet of *P* separates at most one of the 4 corners



⁵Details: Benjamin Müller, Felipe Serrano, Ambros Gleixner, Using two-dimensional Projections for Stronger Separation and Propagation of Bilinear Terms, 2019, ZIB-Report 19-15

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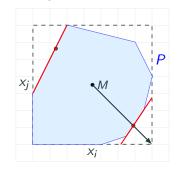
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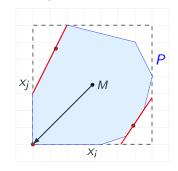
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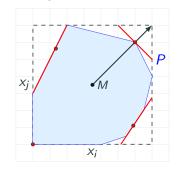
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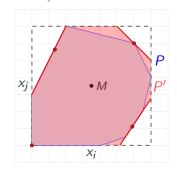
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- \Rightarrow $P' \supseteq P$ described by at most
 - 4 nontrivial inequalities
 - 4 axis-parallel inequalities



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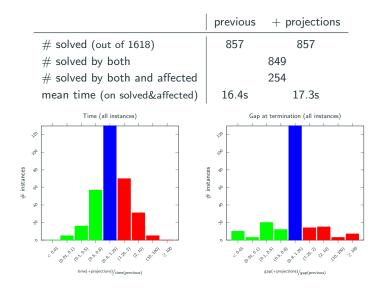
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- x_j M P'
- close connections to optimization-based bound tightening (project LP onto one variable) [Gleixner and Weltge, 2013]
- projections also used to improve bound tightening on x_ix_j

⁵Details: Benjamin Müller, Felipe Serrano, Ambros Gleixner, Using two-dimensional Projections for Stronger Separation and Propagation of Bilinear Terms, 2019, ZIB-Report 19-15

Impact of computing and utilizing 2D projections



Linearizations of products of binary variables

Linearize

$$\prod_{i=1}^n x_i, \qquad x_i \in \{0,1\}:$$

- replace by a new variable $z \in \{0, 1\}$
- if n = 2, add linear constraints $z \le x_1$, $z \le x_2$, $z \ge x_1 + x_2 1$
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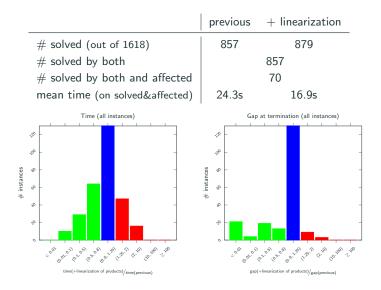
Linearize

$$y \sum_{j=1}^{n} a_j x_j, \qquad x_j \in \{0,1\}, \qquad n \ge 50:$$

- replace by a new variable $z \in \{0, 1\}$, and
- add linear constraints

$$egin{aligned} \mathcal{M}^L y &\leq z \leq \mathcal{M}^U y, \ \sum_j a_j x_j - \mathcal{M}^U (1-y) &\leq z \leq \sum_j a_j x_j - \mathcal{M}^L (1-y). \end{aligned}$$

Impact of linearization of products of binary variables

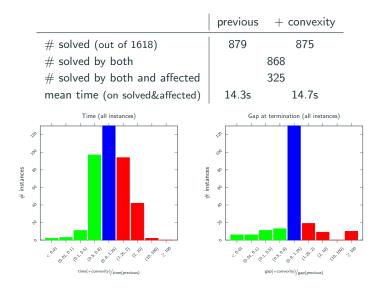


• analyze expressions using a set of rules, e.g.,

$$\begin{split} f(x) \ \text{convex} \Rightarrow \ a \cdot f(x) \begin{cases} \text{convex}, & a \ge 0\\ \text{concave}, & a \le 0 \end{cases} \\ f(x), g(x) \ \text{convex} \Rightarrow \ f(x) + g(x) \ \text{convex} \\ f(x) \ \text{concave} \Rightarrow \ \log(f(x)) \ \text{concave} \end{cases} \\ f(x) = \prod_{i} x_{i}^{e_{i}}, x_{i} \ge 0 \Rightarrow \ f(x) \begin{cases} \text{convex}, & e_{i} \le 0 \ \forall i \\ \text{convex}, & \exists j : e_{i} \le 0 \ \forall i \ne j; \ \sum_{i} e_{i} \ge 1 \\ \text{concave}, & e_{i} \ge 0 \ \forall i; \ \sum_{i} e_{i} \le 1 \end{cases} \end{split}$$

- find maximal convex subexpressions
- underestimate via gradient-cuts

Impact of convexity detection



"On/off"-terms

Given f(x) convex with x semicontinuous, i.e., there exists binary variable y such that

$$x = x_0$$
, if $y = 0$,
 $x \in [\ell, u]$, if $y = 1$.

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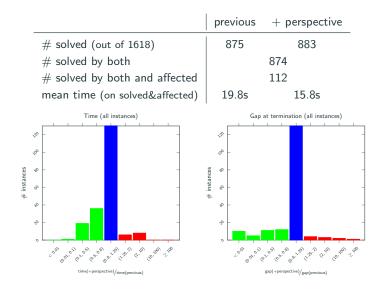
For $x_0 = 0$, f(0) = 0, the perspective cut [Frangioni, Gentile, 2006] $f(\hat{x})y + \nabla f(\hat{x})(x - \hat{x}y) \le w$

is valid for the disjunctive set

$$\{(x, y, z) : x = x_0, y = 0, f(x_0) \le w\} \cup \{(x, y, z) : x \in [\ell, u], y = 1, f(x) \le w\}.$$



Impact of perspective cuts



Symmetry detection

Example:

$$\max x_1 + x_2 + x_3 \\ \text{s.t. } x_1 + x_2 \ge 2 \\ \sqrt{x_1^2 + x_2^2 + x_3^2} \le 5$$

Observation: For any feasible solution, exchanging x_1 and x_2 provides a new feasible solution with same objective value.

Symmetry detection

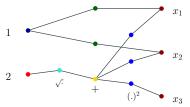
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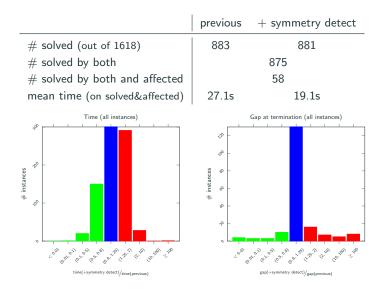
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• can be detected by finding automorphisms on a vertex-colored graph [Liberti 2010]



• SCIP aims to find and break symmetries on binary variables [SCIP 5 report, 2017]

Impact of symmetry



A new framework for NLP in SCIP (work in progress)

Conclusion

The handling of nonlinear constraints in SCIP is rewritten.

The new code will be nicer, better, faster, greater:

- less issues with slightly infeasible solutions
- easier to extend by own operators and structure-exploiting algorithms

Core: new constraint handler (cons_expr)

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Nonlinearity Handler:

- quadratic: recognize and separate convex quadratic; domain propagation
- bilinear: tighter estimators and bounds for $x_i x_j$ over polytope
- convex: recognize some simple general convexities, separate by linearization
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Symmetry detection

Not ready yet, but getting closer

