Nonlinear constraints in SCIP

Ksenia Bestuzheva and Stefan Vigerske

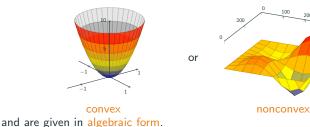
SCIP Online Workshop 2020 \cdot June 3, 2020

Mixed-Integer Nonlinear Programming

min
$$c^T x$$

s.t. $g_k(x) \le 0$ $\forall k \in [m]$
 $x_i \in \mathbb{Z}$ $\forall i \in \mathcal{I} \subseteq [n]$
 $x_i \in [\ell_i, u_i]$ $\forall i \in [n]$

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



200

-200

• SCIP solves MINLPs by spatial Branch & Bound.

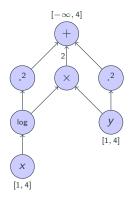
The "classical" framework for (MI)NLP in SCIP

Expression trees and graphs

cons_nonlinear stores algebraic structure of nonlinear constraints in one directed acyclic graph:

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

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



Expression trees and graphs

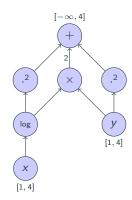
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- nodes: variables, operations, constraints
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Operators:

- 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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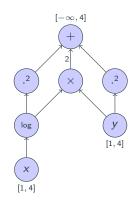
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- exp, log
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- ∑, ∏, affine-linear, quadratic, signomial
- (user)

Additional constraint handler: quadratic, abspower $(x \mapsto x|x|^{p-1}, p > 1)$, SOC

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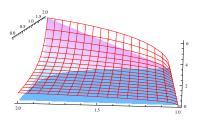
Reformulation in cons_nonlinear (during presolve)

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

Example:

$$g(x) = \sqrt{\exp(x_1^2) \ln(x_2)}$$

 $x_1 \in [0, 2], \quad x_2 \in [1, 2]$



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

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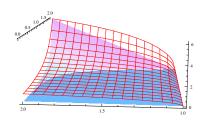
$$g = \sqrt{y_1}$$

$$y_1 = y_2 y_3$$

$$y_2 = \exp(y_4)$$

$$y_3 = \ln(x_2)$$

$$y_4 = x_1^2$$



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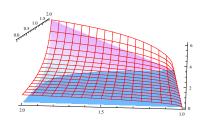
$$g = \sqrt{y_1}$$

$$y_1 = y_2 y_3 \qquad [0, \ln(2)e^4]$$

$$y_2 = \exp(y_4) \qquad [1, e^4]$$

$$y_3 = \ln(x_2) \qquad [0, \ln(2)]$$

$$y_4 = x_1^2 \qquad [0, 4]$$



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Bounding: LP relaxation

- relaxing integrality
- convexifying non-convexities
- linearizing nonlinear convexities

convex functions concave functions

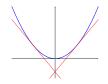


 $x^k \quad (k \in 2\mathbb{Z} + 1)$



 $x \cdot y$



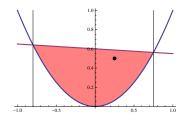


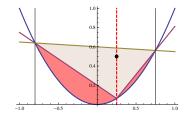


Branching

- 1. fractional integer variables
- 2. variables in violated nonconvex constraints, because variable bounds determine the convex relaxation, e.g.,

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





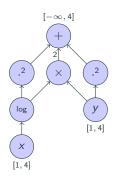
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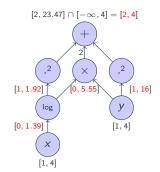
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- Forward propagation:
 - compute bounds on intermediate nodes (top-down)



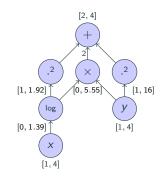
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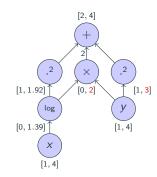
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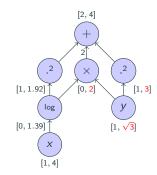
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Further Techniques

Primal Heuristics:

- NLP solving: subnlp, nlpdiving, multistart, mpec
- MINLP solving: LNS heuristics (RENS, RINS, DINS, etc.)
- MIP solving: undercover

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Tighter Relaxations:

- second-order cone upgrade of quadratic constraints
- adding KKT reformulation (using SOS1) for QPs
- $x \cdot y$ over 2D projections of the LP relaxation
- separation for edge-concave quadratic constraints (off by default)
- projection of LP relaxation onto convex feasible sets (off by default)

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More Bound Tightening:

- Optimization-Based Bound Tightening: min / max x_i w.r.t. LP relaxation
- nl. Optimization-Based Bound Tightening: min / max x_i w.r.t. convex NLP relaxation (off by default)

Interfaces

A MINLP can be input via

- File readers: FlatZinc*, LP*, MPS*, OSiL, PIP†, ZIMPL
- Interfaces: AMPL, C, GAMS, Java*, Julia/JuMP, Matlab (via OPTI Toolbox), Python

SCIP can utilize this software for MINLP solving:

- NLP Solvers: Ipopt, FilterSQP, WORHP
- Automatic Differentiation: CppAD

^{*} quadratic only

[†]polynomial only



Stefan, you need to switch screen to Ksenia now.

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

by K. Bestuzheva, B. Müller, F. Serrano, S.

Vigerske, F. Wegscheider

Problem with current implementation

Consider

 $\min z$

s.t.
$$\exp(\ln(1000) + 1 + xy) \le z$$

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

An optimal solution:

$$x = -1$$

$$y = 1$$

$$z = 1000$$

Problem with current implementation

```
An optimal solution:
                  \min z
                                                             x = -1
Consider
                  s.t. \exp(\ln(1000) + 1 + xy) < z
                                                      v = 1
                      x^2 + y^2 \le 2
                                                            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
                     : 0.00 %
Gap
  [nonlinear] \langle e1 \rangle: exp((7.9077552789821368151 +1 (<math>\langle x \rangle * \langle y \rangle)))-1 \langle z \rangle[C] \langle e \rangle
violation: right hand side is violated by 0.000673453314561812
best solution is not feasible in original problem
                                        -1.00057454873626
                                                              (obj:0)
х
                                        0.999425451364613
                                                              (obj:0)
у
                                         999.999656552061
                                                              (obj:1)
\mathbf{z}
```

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

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

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

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

Violation

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

$$0.6731\cdot 10^{-6} \leq ext{numerics/feastol} \, \checkmark$$

$$0.6602 \cdot 10^{-6} \leq \texttt{numerics/feastol} \; \checkmark$$

Solution (found by <relaxation>):

x = -1.000574549

y = 0.999425451

z = 999.999656552

w= 6.907754936

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min z Violation
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- ⇒ Explicit reformulation of constraints ...
 - ... loses the connection to the original problem.

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- ⇒ 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.

Main Ideas

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}
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- \Rightarrow avoid redundancy / ambiguity of expression types (classic: +, \sum , linear, quad., . . .)
 - stronger identification of common subexpressions

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Do not reformulate constraints.

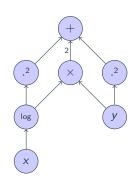
introduce auxiliary variables for the relaxation only

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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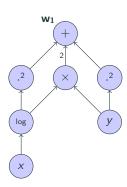
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(Implicit) Reformulation:

$$w_1 \le 4$$

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



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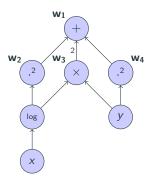
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 $w_2 + 2w_3 + w_4 = w_1$
 $\log(x)^2 = w_2$
 $\log(x)y = w_3$
 $y^2 = w_4$



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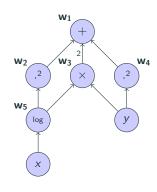
$$w_2 + 2w_3 + w_4 = w_1$$

$$w_5^2 = w_2$$

$$w_5 y = w_3$$

$$y^2 = w_4$$

$$\log(x) = w_5$$



Enforcement

Constraint:

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- presolve,
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$$y^2 = w_4$$

$$\log(x) = w_5$$

W₁

Used to construct LP relaxation.

Expression handler

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
- 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):
O deleted vars, O 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 <nonlinear>
[...]
SCIP Status
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min z s.t. \exp(\ln(1000) + 1 + xy) \le z, x^2 + y^2 \le 2
```

Classic: New:

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                                                              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
                                                               0 implications, 0 cliques
presolved problem has 4 variables (0 bin, 0 int, 0 impl, 4 ponts) lved problem has 3 variables (0 bin, 0 int, 0 impl, 3 cont)
  and 3 constraints
                                                                and 2 constraints
      2 constraints of type <quadratic>
                                                                    2 constraints of type <expr>
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[...]
                                                              ſ...1
SCIP Status
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                                                              Solving Time (sec): 0.47
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Solving Nodes
                                                              Solving Nodes
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                                                                                  : +9.99999949950021e+02 (2 solutions)
Dual Round
                    · +9 99999656552062e+02
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                                       999.999656552061 (objz1)
                                                                                                                        (obj:1)
```

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 $(\log(x), y)$.

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 $(\log(x), y)$.
- \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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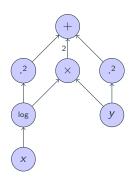
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Nonlinearity Handler (nlhdlrs):

- 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.
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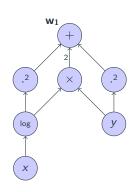


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Constraint:
$$\log(x)^2 + 2\log(x)y + y^2 \le 4$$

$$w_1 \le 4$$

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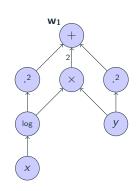


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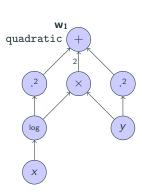


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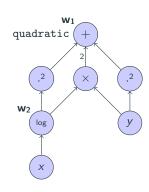
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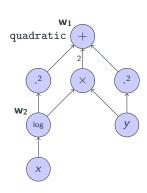
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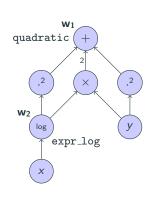
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$$w_1 \le 4$$
 $w_2^2 + 2w_2y + y^2 \le w_1$ [nlhdlr_quadratic] $\log(x) = w_2$ [expr_log]

- 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.



Current status

Available features:

- Handler for quadratic subexpressions
- Handler for second-order cone structures
- Handler for convex and concave subexpressions
- Handler for functions on semi-continuous variables (perspective formulations)
- Handler for bilinear terms $(x \cdot y \text{ over 2D projection of LP relaxation})$
- RLT (Reformulation-Linearization Technique) separator for bilinear terms
- Separator for SDP cuts on 2×2 principal minors of $X xx^T \succeq 0$
- Linearization of products of binary variables
- Symmetry detection
- Support for operators cos, sin, entropy
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Main open tasks before release:

- check performance "outliers"
- replacing remaining classic code by new one (in particular NLP relaxation and NLP solver interfaces)
- documentation "?"

Nonlinear constraints in SCIP

Ksenia Bestuzheva and Stefan Vigerske SCIP Online Workshop 2020 · June 3, 2020