Undercover

A primal heuristic for MINLP based on sub-MIPs generated by set covering

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joint work with Ambros M. Gleixner

DFG Research Center MATHEON
Mathematics for key technologies

1. Introduction: MINLP & primal heuristics
2. A generic algorithm for Undercover
3. Finding minimum covers
4. Computational environment and experiments
5. Extensions: fix-and-propagate etc.
6. Conclusion

Outline

Mixed Integer Linear Program

Objective function:

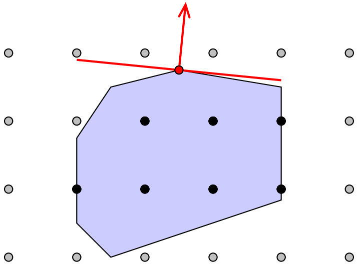
▷ linear function

Feasible set:

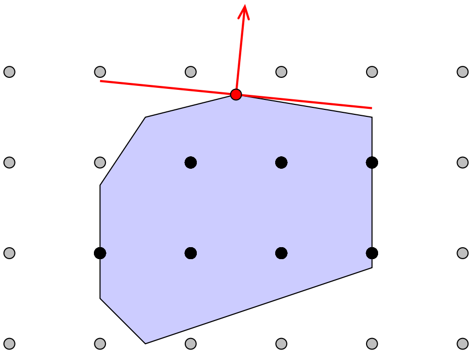
▷ described by linear constraints

Variable domains:

▷ real or integer values

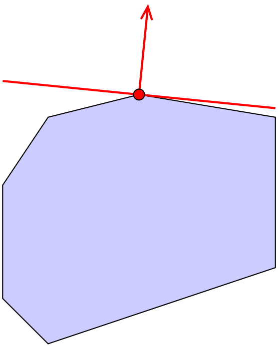


$$\begin{aligned} \min\ & c^T x && c \in \mathbb{R}^n \\ \text{s. t. } & Ax \leqslant b && A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m \\ & x_i \in \mathbb{Z} && i \in \mathcal{I} \subseteq \{1, \ldots, n\} \end{aligned}$$



Important terms

- LP relaxation
- LP-based branch-and-bound
- feasible solutions
- optimal solutions



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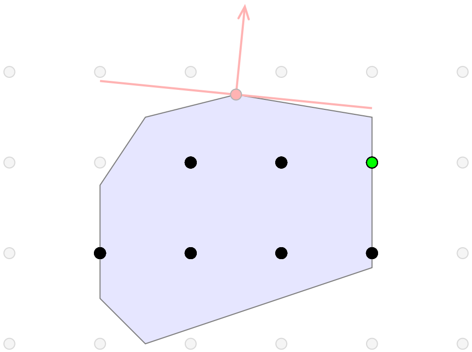
What is Mixed-Integer Linear Programming?



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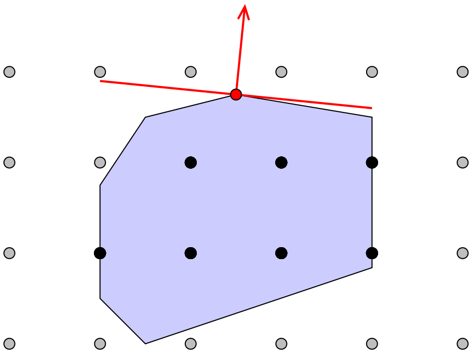

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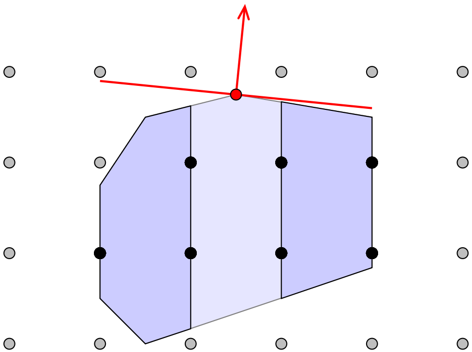

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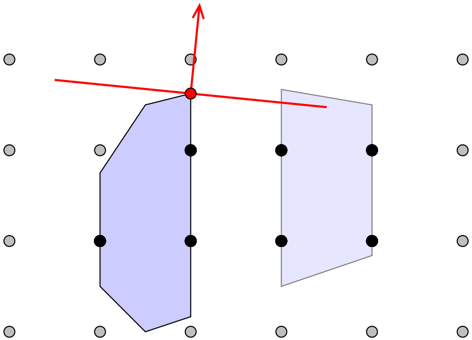

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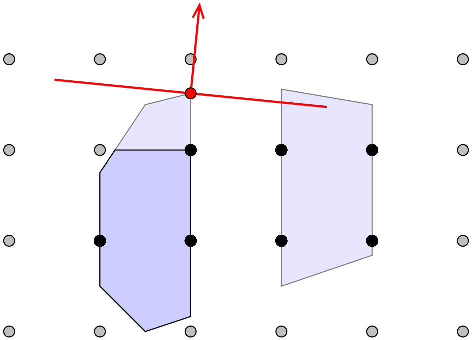

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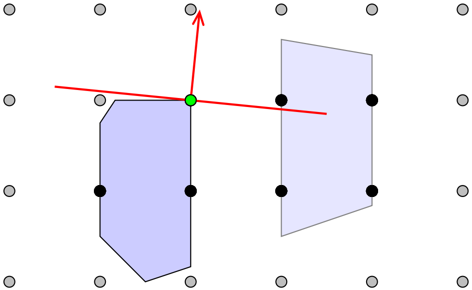

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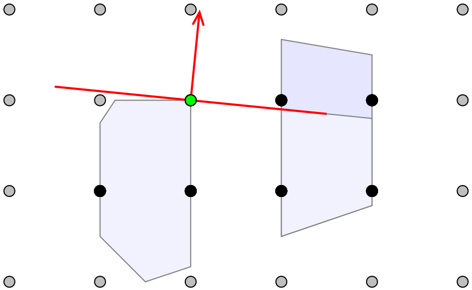

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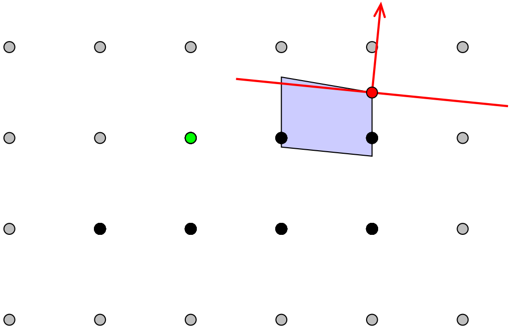

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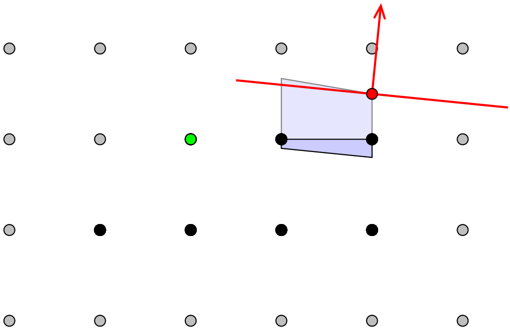

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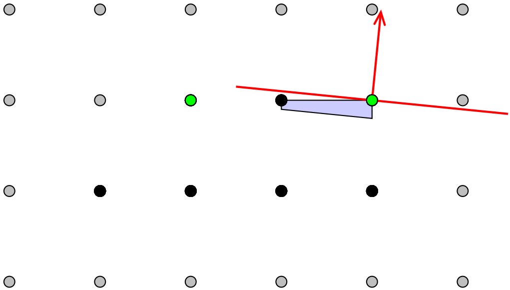

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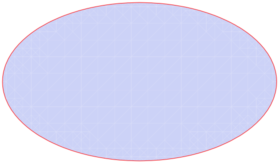
What is Mixed-Integer Nonlinear Programming?

$$\begin{aligned} \min\ & c^T x & & c \in \mathbb{R}^n \\ \text{such that } & g(x) \leqslant 0, & & g \in C^1(\mathbb{R}^n, \mathbb{R}^m) \\ & x_i \in \mathbb{Z}, \quad i \in \mathcal{I}. & & \mathcal{I} \subseteq \{1, \dots, n\} \end{aligned}$$

MINLP is difficult due to combination of

- nonlinearity $\quad x_1^2 + 3x_2^2 \leqslant 3$



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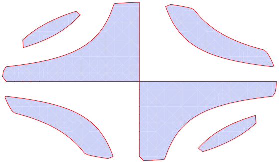
MINLP is difficult due to combination of

- nonlinearity $x_1^2 + 3x_2^2 \leqslant 3$
- nonconvexity $\sin(10x_1x_2) \leqslant 0$



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\end{aligned}
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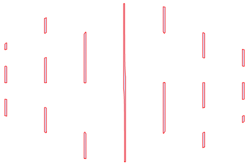
MINLP is difficult due to combination of

- ▷ nonlinearity $x_1^2 + 3x_2^2 \leqslant 3$
- ▷ nonconvexity $\sin(10x_1x_2) \leqslant 0$
- ▷ integrality $x_1 \in \mathbb{Z}$



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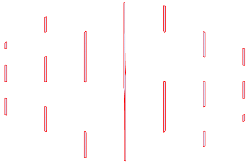


Important subclass: convex MINLP
MINLP is convex $\Leftrightarrow$ each function $g_j : \mathbb{R}^n \to \mathbb{R}$ is convex

Applications in many areas, e.g.,

- engineering design: e.g., mining with stockpiling constraints
- manufacturing: e.g., sheet metal design
- chemical industry: e.g., design of synthesis processes
- networks: operation and design of water and gas networks
- energy production and distribution: e.g., plant design, power scheduling
- logistics: e.g., public transport
- ...





$$\begin{aligned} \min \quad & c^T x \\ \text{such that} \quad & g(x) \leqslant 0 \\ & x_i \in \mathbb{Z}, \quad i \in \mathcal{I} \end{aligned}$$

Assumption: $g : \mathbb{R}^n \to \mathbb{R}^m$ is convex, each g_j continuously differentiable

NLP based branch–and–bound

▷ bounding: solve convex nonlinear relaxation (NLP)

$$\begin{aligned} \min \quad & c^T x \\ \text{such that} \quad & g(x) \leqslant 0 \end{aligned}$$

▷ branching: on integer variables with fractional LP value

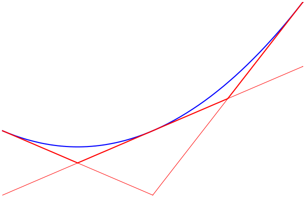
LP based branch–and–cut

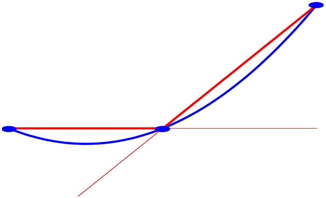
▷ bounding: solve polyhedral outer-approximation (LP)

$$\tilde{x} = \operatorname{argmin} \quad c^T x$$
$$\text{such that} \quad g_j(\hat{x}) + \nabla g_j(\hat{x})(x - \hat{x}) \leqslant 0, \quad j = 1, \dots, m, \quad \hat{x} \in S$$

If $g(\tilde{x}) > 0$, add supporting hyperplane to LP, i.e., add $\tilde{x}$ to S.

▷ branching: on integer variables with fractional LP value





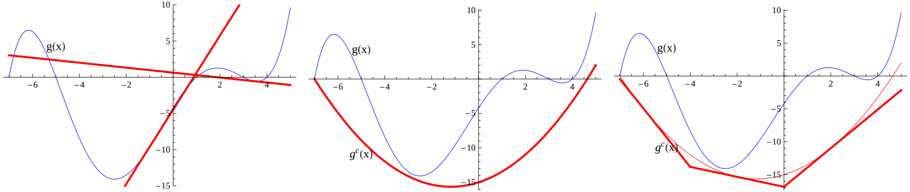
$$\begin{aligned} \min \quad & c^T x \\ \text{such that} \quad & g(x) \leqslant 0 \\ & x_i \in \mathbb{Z}, \quad i \in \mathcal{I} \end{aligned}$$

Now: some components of $g : \mathbb{R}^n \to \mathbb{R}^m$ may be nonconvex

$\Rightarrow$ inequalities $g_j(\hat{x}) + \nabla g_j(\hat{x})(x - \hat{x}) \leqslant 0$ may not be valid!

$\Rightarrow$ use convex underestimator: convex and below $g(x)$ for all $x \in [L, U]$

$\Rightarrow$ introduces convexification gap



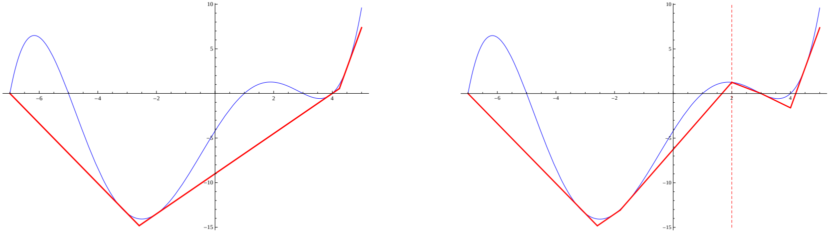
Spatial branch–and–bound

- **bounding:** solve polyhedral outer-approximation

$$
\begin{aligned}
\min \quad & c^T x \\
\text{such that} \quad & g_j^c(\hat{x}) + \nabla g_j^c(\hat{x})(x - \hat{x}) \leqslant 0, \quad j = 1, \ldots, m, \quad \hat{x} \in S, \\
& x \in [L, U]
\end{aligned}
$$

- **branching**: close gap between relaxation and problem
  - on integer variables with fractional value in LP relax
  - on continuous variables in nonconvex terms

    ⇒ tighter bounds ⇒ better underestimators



Finding feasible solutions. . .

- wait for the LP relaxation to become feasible
- MIP heuristics applied to LP
  - rounding, diving, feasibility pump,. . .
- extend MIP heuristics to MINLP
- MINLP specific heuristics → this talk

Why use primal heuristics inside an exact solver?

- Able to prove feasibility of the model
- Often nearly optimal solutions suffice in practice
- Feasible solutions guide remaining search process

Source		convex	nonconvex
MIP heuristics for linear outer approximations		✓	✓
NLP local search with fixed integralities		✓	✓
Simple NLP Rounding		✓	✓
Fractional Diving & Vectorlength Diving			
	BonamiGonçalves08	✓	(✓)
Iterative Rounding	NanniciniBelotti	✓	✓
FeasPump	BonamiCornuéjolsLodiMargot08	✓	nonconvex obj. convex feas. region
	D'AmbrosioFrangioniLibertiLodi09	✓	✓
	LinderothAbhishekLeyfferSartenaer08	✓	
Local Branching	NanniciniBelottiLiberti08	✓	✓
RECIPE	LibertiNanniciniMladenović08	✓	✓
RENS	BertholdHeinzVigerske09 (for MIQCPs)	✓	✓

⋮

- LNS: common paradigm in MIP heuristics

  fix a subset of variables $\rightsquigarrow$ easy subproblem $\rightsquigarrow$ solve

  MIP: “easy” $=$ few integralities MINLP: “easy” $=$ few nonlinearities

- Observation: Any MINLP can be reduced to a MIP by fixing (sufficiently many) variables.

  Experience: Often, few fixings are sufficient!

- Idea: Fix a small subset of variables to obtain a linear subproblem (MIP).
- Use solution of a LP or NLP relaxation to determine fixing values

Definition (cover of a function)

Let

- a function $g : D \to \mathbb{R}$, $x \mapsto g(x)$ on a domain $D \subseteq \mathbb{R}^n$,
- a point $x^\star \in D$, and
- a set $\mathcal{C} \subseteq \{1, \ldots, n\}$ of variable indices be given.

We call $\mathcal{C}$ an *$x^\star$-cover of g* if and only if the set

$$\{(x, g(x)) \mid x \in D, x_k = x_k^\star \text{ for all } k \in \mathcal{C}\} \tag{1}$$

is affine.

We call $\mathcal{C}$ a *(global) cover of g* if and only if $\mathcal{C}$ is an $x^\star$-cover of g for all $x^\star \in D$.

Definition (cover of an MINLP)

Let

- P be an MINLP
- $x^\star \in [L, U]$, and
- $\mathcal{C} \subseteq \{1, \ldots, n\}$ be a set of variable indices of P.

We call $\mathcal{C}$ an *$x^\star$-cover of P* if and only if $\mathcal{C}$ is an $x^\star$-cover for $g_1, \ldots, g_m$.

We call $\mathcal{C}$ a *(global) cover of P* if and only if $\mathcal{C}$ is an $x^\star$-cover of P for all $x^\star \in [L, U]$.

A generic algorithm

Input: MINLP P

begin

compute a solution $x^\star$ of an approximation of P

round $x^\star_k$ for all $k \in \mathcal{I}$

determine an $x^\star$-cover $\mathcal{C}$ of P

solve the sub-MIP of P given by fixing $x_k = x^\star_k$ for all $k \in \mathcal{C}$

end

A generic algorithm

```
Input: MINLP P
begin
    compute a solution x* of an approximation of P
    round x*_k for all k ∈ I
    determine an x*-cover C of P
    solve the sub-MIP of P given by fixing x_k = x*_k for all k ∈ C
end
```

Input: MINLP P
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Remark:

- MIP heuristics: trade-off fixing many vs. few variables

  Here: Eliminate nonlinearities by fixing as few as possible variables $\rightarrow$ minimum $x^\star$-cover!

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Remark:

- MIP heuristics: trade-off fixing many vs. few variables

  Here: Eliminate nonlinearities by fixing as few as possible variables $\rightarrow$ minimum $x^\star$-cover!
- How to find minimum cover?

Let $g : \mathbb{R}^n \to \mathbb{R}, x \mapsto x^T Qx + qx + c,\ Q \in \mathbb{R}^{n\times n}$ symmetric, $x^\star \in \mathbb{R}^n$.

Fixing variables with indices in $\mathcal{C} \subseteq \{1, ..., n\}$ transforms

$$x^T Qx \quad \overset{x_k = x_k^\star\ \forall k \in \mathcal{C}}{\rightsquigarrow} \quad y^T \tilde{Q} y + \tilde{q}^T y + \tilde{c}$$

with $y = (x_k)_{k \notin \mathcal{C}} \in \mathbb{R}^{n-|\mathcal{C}|}$, and $\tilde{Q} = (Q_{uv})_{u,v \notin \mathcal{C}} \in \mathbb{R}^{(n-|\mathcal{C}|)\times(n-|\mathcal{C}|)}$, ...

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Thus: $\mathcal{C}$ is a cover of g iff

$q_{uv} = 0$ for all $u, v \notin \mathcal{C}$

independent of fix. values.

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$\leftrightsquigarrow$

set covering:

cover nonzeros in Q by incident rows/columns

$$\begin{pmatrix} & * & & & \\ * & * & * & & \\ & * & & * & * \\ & & * & & \\ & & * & & \end{pmatrix}$$

Covering quadratic functions

Let $g : \mathbb{R}^n \to \mathbb{R}, x \mapsto x^T Qx + qx + c,\ Q \in \mathbb{R}^{n\times n}$ symmetric, $x^\star \in \mathbb{R}^n$.

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$q_{uv} = 0$ for all $u, v \notin \mathcal{C}$ $\quad\leftrightsquigarrow\quad$ **set covering:** cover nonzeros in Q by incident rows/columns

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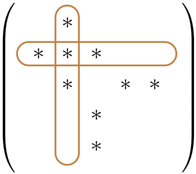

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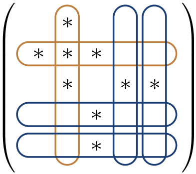

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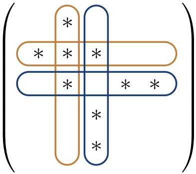
$q_{uv} = 0$ for all $u, v \notin \mathcal{C}$ $\quad\leftrightsquigarrow$

independent of fix. values.

set covering:

cover nonzeros
in Q by incident
rows/columns



Auxiliary binary variables:

$$\alpha_k = 1 :\Leftrightarrow x_k \text{ is fixed in } P$$

Set Covering constraints:

$\mathcal{C}(\alpha) := \{k \mid \alpha_k = 1\}$ is a cover of P if and only if

$$\alpha_k = 1 \qquad \text{for all square nonzeros: } Q^i_{kk} \neq 0, \tag{2}$$

$$\alpha_k + \alpha_j \geqslant 1 \qquad \text{for all bilinear nonzeros: } Q^i_{kj} \neq 0, k \neq j. \tag{3}$$

To find a minimum cover, we solve the covering problem

$$\min \Big\{ \sum_{k=1}^{n} \alpha_k : (2), (3), \alpha \in \{0,1\}^n \Big\}. \tag{4}$$

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- (4) is an $\mathcal{NP}$-hard problem, but standard branch-and-cut is (empirically) very fast.

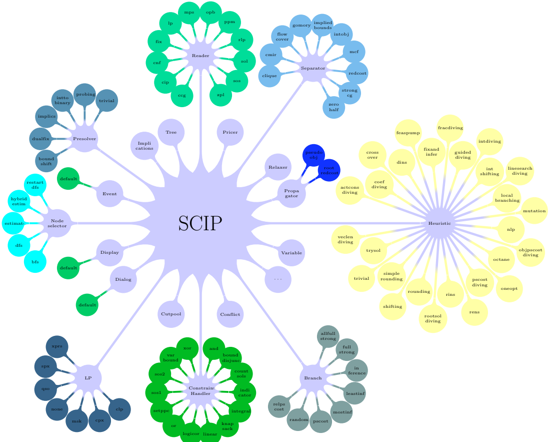
- For general MINLPs, the covering problem becomes more difficult, e.g. for a global cover of a monomial $x_1^{p_1} \cdots x_n^{p_n}$, $p_1, \ldots, p_n \in \mathbb{N}_0$:

$$\alpha_k = 1 \qquad \text{for all } p_k \geqslant 2$$

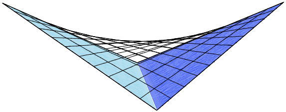
$$\sum_{k:p_k=1} (1 - \alpha_k) \leqslant 1.$$

- For general MINLPs, global covers become larger and larger. *However:* $x^\star$-covers are a weaker notion, may be significantly smaller

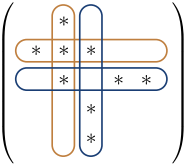
- a branch-cut-and-price framework
- incorporates CP, MIP, and SAT-solving features
- provides full-scale MIP solver
- modular structure via plugins
- free for academic purposes, `http://scip.zib.de`



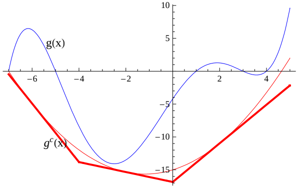
SCIP has recently been extended to handle nonconvex MIQCPs
$\Rightarrow$ all nonlinear constraints are of quadratic form $g_i(x) = x^T A_i x + b_i^T x + c_i$



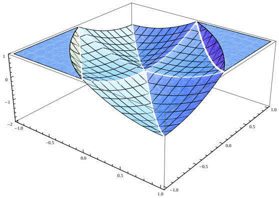
McCormick



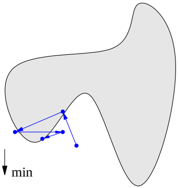
Undercover



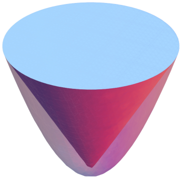
Convexification



Geometric branching

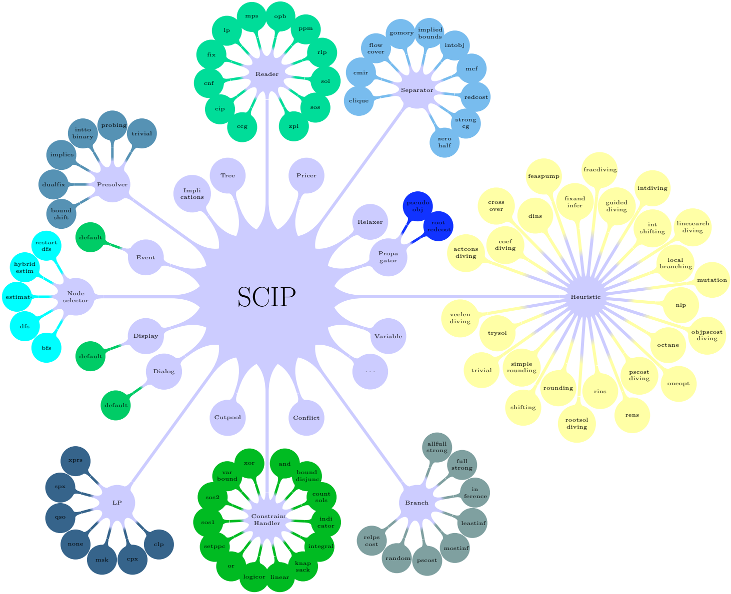


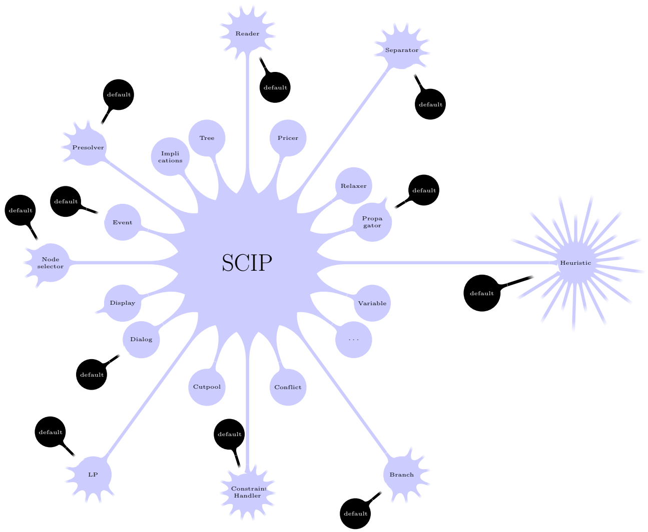
NLP local search



Second Order Cone

SCIP: MIQCP Plugins




SCIP
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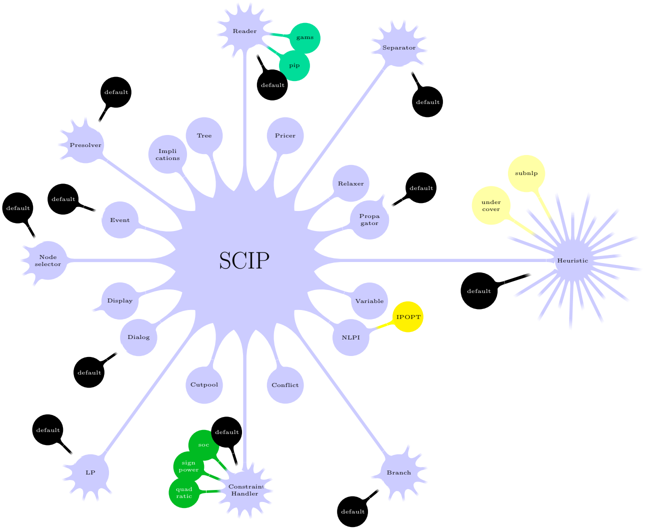
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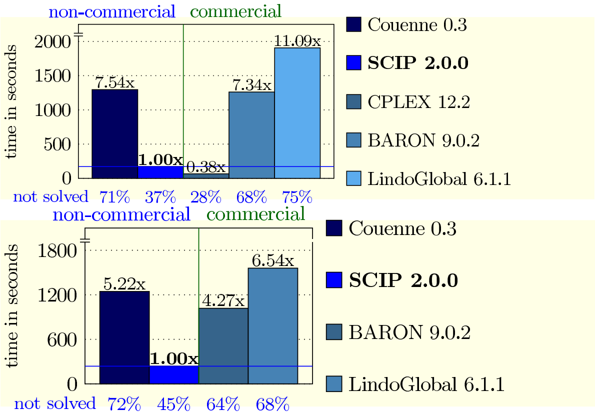
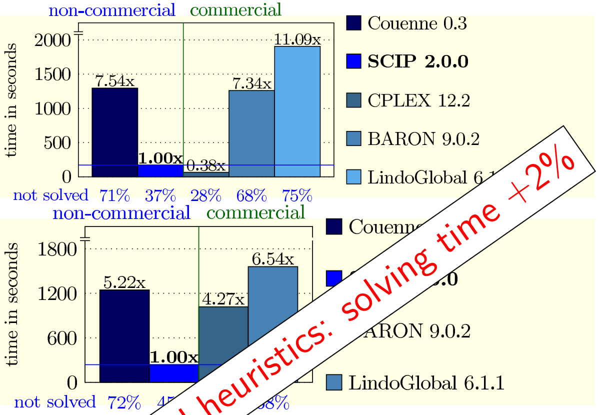


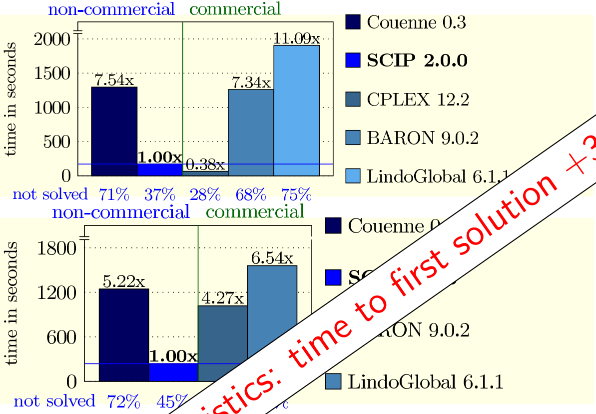
- 94 publicly available instances from 7 sources
- SCIP uses Cplex as LP solver and Ipopt as NLP solver
- 1 hour time limit

SCIP: Computational Results



- 94 publicly availabl… …nces from 7 sources
- SCIP uses Cpl… …P solver and Ipopt as NLP solver
- 1 hour tim… …t

Impact primal heuristics: solving time +2%



Impact primal heuristics: time to first solution +347%

- 94 publicly available … ces from 7 sources
- SCIP uses Cple… solver and Ipopt as NLP solver
- 1 hour tim…

▷ Goal
- evaluate potential as start heuristic at the root node

▷ Test set
- 33 MIQCP instances from MINLPLib

▷ Undercover parameters
- running as only root node heuristic in SCIP
- for sub-MIP: emphasis feasibility and fast presolving settings

▷ Reference solvers
- SCIP 1.2.1.1
- BARON 9.02
- Couenne 0.2
- default, node limit 1

▷ Reported
- nonlinear nonzeros/variable
- % variables fixed by Undercover
- solution values of each solver
- best known solution

12 instances with ⩽ 5% variables fixed

instance	nnz/var	% cov	UC	SCIP	BARON	Couenne	known
netmod_dol1	0.00	0.30	0	**-0.26321**	0	–	-0.56
netmod_dol2	0.00	0.38	-0.07802	**-0.50562**	0	–	-0.56
netmod_kar1	0.01	0.88	**0**	**0**	**0**	–	-0.4198
netmod_kar2	0.01	0.88	**0**	**0**	**0**	–	-0.4198
space25	0.12	1.04	–	–	–	–	484.33
ex1266	0.40	3.03	**16.3**	–	–	–	16.3
util	0.07	3.13	**999.58**	1000.5	1006.5	–	999.58
feedtray2	10.70	3.26	–	–	**0**	–	0
ex1265	0.38	3.52	**15.1**	–	–	**15.1**	10.3
ex1263	0.34	3.88	**30.1**	–	–	–	19.6
tln12	1.70	3.99	–	–	–	–	90.5
ex1264	0.36	4.26	**11.1**	–	–	–	8.6

- ▷ 9 instances feasible, 7 times best solution value
- ▷ `ex1266` and `util` optimal

10 instances with 5–15% variables fixed

instance	nnz/var	% cov	UC	SCIP	BARON	Couenne	known
waste	1.10	5.65	**608.76**	–	712.301	–	598.92
space25a	0.29	5.84	–	–	–	–	484.33
nuclear14a	4.98	6.43	–	–	–	–	-1.1280
nuclear14b	2.42	6.43	–	–	–	**-1.1105**	-1.1135
tln7	1.53	6.67	**30.3**	–	–	–	15
tln6	1.47	7.69	**20.3**	–	–	–	15.3
tloss	1.47	7.89	**16.3**	–	–	–	16.3
tln5	1.39	9.09	15.1	–	–	**14.5**	10.3
sep1	0.40	10.53	**-510.08**	–	**-510.08**	**-510.08**	-510.08
tltr	1.10	12.50	**74.2**	–	–	–	48.067

- 7 instances feasible, 6 times best solution value
- `tloss` and `sep1` optimal

11 instances with 15–96% variables fixed

instance	nnz/var	% cov	UC	SCIP	BARON	Couenne	known
nous1	2.39	19.44	–	–	–	**1.5671**	1.5671
nous2	2.39	19.44	–	1.3843	**0.62597**	1.3843	0.626
meanvarx	0.19	23.33	15.925	**14.369**	**14.369**	18.702	14.369
product2	0.37	26.15	–	–	–	–	-2102.4
product	0.17	30.87	–	–	–	–	-2142.9
spectra2	3.43	35.71	31.981	**13.978**	119.87	–	13.978
fac3	0.81	78.26	13065	**7213**	38329	–	3198
nvs19	8.00	88.89	–	0	**-1098**	–	-1098.4
nvs23	9.00	90.00	–	0	**-1124.8**	–	-1125.2
du-opt5	0.95	94.74	3407.1	**14.168**	–	1226.0	8.0737
du-opt	0.95	95.24	4233.9	4233.9	108.33	**41.304**	3.5563

▷ 5 instances feasible, no best solution value

- Feasible solutions
  - Undercover: 21 instances
  - SCIP: 13 instances
  - BARON: 15 instances
  - Couenne: 9 instances
  - All: 27 instances

- Solution quality
  if both found a solution
  - Undercover : SCIP = 1:6 (2 equal)
  - Undercover : BARON = 5:2 (3 equal)
  - Undercover : Couenne = 1:3 (2 equal)

- Undercover time always < 0.2 seconds (except for `waste` with 1.1 sec)
  - covering problem always solved to optimality at root
  - most time spent in sub-MIP
  - 20 of 21 feasible sub-MIPs solved to optimality
  - infeasibility of sub-MIP usually detected in advance (10 of 12)

Outline

Fix-and-propagate

- Do not fix variables in $\mathcal{C}$ simultaneously, but sequentially and propagate after each fixing.
- If $x_k^\star$ falls out of bounds then
  - fix to the closest bound (similar to FischettiSalvagnin09)
  - recompute the approximation

Backtracking

- If fix-and-propagate deduces infeasibility, apply a one-level backtracking: undo last fixing and try another value

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Using different covers

Covers minimising different impact measures

- minimum cardinality covers: minimise impact on MINLP

- Alternative impact measures as objective function of covering problem:
  - appearance in nonlinear terms
  - appearance in violated nonlinear constraints
  - domain size
  - variable type
  - rounding locks on integer variables
  - hybrid measures

- In particular: if a minimum cardinality cover yields infeasible sub-MIP

Covers minimising different impact measures

- minimum cardinality cov : on MINLP
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  - appearance in violated n
  - domain size
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Recovering

- fix-and-propagate may fix variables outside the cover $\mathcal{C}$
- $\leadsto$ variables in $\mathcal{C}$ might not need to be fixed

  $\leadsto$ "re-cover": solve the covering problem again with propagated bounds

Recovering

- fix-and-propagate may fix va … le the cover $\mathcal{C}$
- $\rightsquigarrow$ variables in $\mathcal{C}$ might not … ‹ed

  $\rightsquigarrow$ "re-cover": solve the cov … ı again with propagated bounds

NLP postprocessing

- All sub-MIP solutions are fully feasible for the original MINLP.
- Still, sub-MIP solution $\tilde{x}$ could be improved by NLP local search:
  - fix all integer variables of the original MINLP to their values in $\tilde{x}$
  - solve the resulting NLP to local optimality

NLP postprocessing

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▷ Still, sub-MIP solution $\tilde{x}$ … by NLP local search:

- fix all integer variables c … o their values in $\tilde{x}$
- solve the resulting NLP

If the sub-MIP is infeasible, this is typically detected

- during fix-and-propagate, or
- via infeasible root LP.

$\rightsquigarrow$ Generate conflict clauses for the original MINLP .

- Add them to the original MINLP.
- Use them to revise fixing values and/or fixing order.
- Start another fix-and-propagate run.

If the sub-MIP remains infeasible, at least this gives us valid conflicts to prune the search tree in the original problem.

Avoiding/exploiting infeasibility

If the sub-MIP is infeasible, this is typically detected

- during fix-and-propagate, or
- via infeasible root

⤳ Generate conflict

- Add them to the o
- Use them to revise r.
- Start another fix-a

If the sub-MIP remains infeasible, at least this gives us valid conflicts to prune the search tree in the original problem.

Variations: convexification & domain reduction

- Idea of Undercover: fix few variables to obtain an “easy” subproblem.
  - switch to easier problem class
  - switch to easier problem of the same class
- Switch to easier problem class:
  - MIQCP $\rightsquigarrow$ MIP
  - MINLP $\rightsquigarrow$ MIQCP
  - nonconvex MINLP $\rightsquigarrow$ convex MINLP
  - ...
- Switch to easier problem of the same class: restrict variable domains
  - significantly better outer approximations
  - leaves more freedom to the problem

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  - ...

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- Scheme of a general-purpose start heuristic for MINLP
  - solve a set covering problem
  - to identify few variable fixings
  - yielding a mixed-integer linear subproblem
- Preliminary experiments
  - MIQCPs from MINLPLib – often few fixings sufficient: $\leqslant 5\%$ on $1/3$ of the test set, $\leqslant 15\%$ on $2/3$ of the test set
  - successfully applied as root node heuristic
- Future research
  - extensions and variations
  - experiments on general MINLPs
  - tuning for efficient use within branch-and-bound tree
  - use NLP relaxation instead of LP outer approximation

Undercover

A primal heuristic for MINLP based on sub-MIPs generated by set covering

Timo Berthold

Zuse Institute Berlin • MATHEON • BMS

joint work with Ambros M. Gleixner

DFG Research Center MATHEON
Mathematics for key technologies