Aspects on Solving Convex and Nonconvex Mixed Integer Nonlinear Programming Problems

Professor Tapio Westerlund

PROCESS DESIGN AND SYSTEMS ENGINEERING LABORATORY
ÅBO AKADEMI UNIVERSITY, TURKU, FINLAND

University of the Witwatersrand, Johannesburg, October 28th 2016

OPTIMIZATION AND SYSTEMS ENGINEERING
Åbo Akademi University

A few words about Åbo Akademi University

The University (ÅAU) was originally founded in 1640.
After a big fire in the town,1828, ÅA moved to Helsinki (as Helsinki University)
ÅAU was re-established in Turku (Åbo) in 1918.

Finland

- population: 5.3 million
- area: 131.000 sq mi
- official languages:
  - Finnish 92%
  - Swedish 6%

Åbo Akademi University

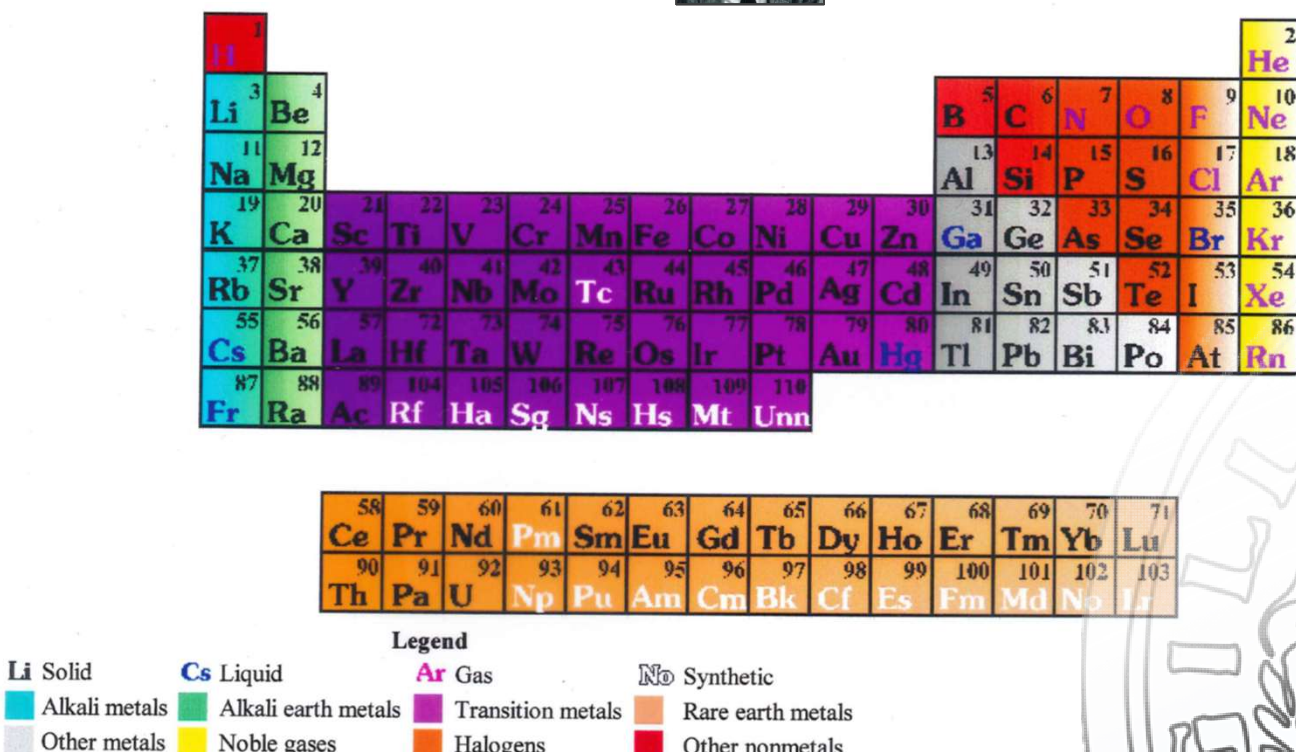
- 7000 students
- multidisciplinary
- education in Swedish

Some names from the history of Åbo Akademi University

1700: Anders Lexell (1740-1784) (mathematics, astronomy) (Successor of Leonhard Euler in St:Petersburg)

1800: Johan Gadolin (1760-1852) (chemistry) (Element 64 Gd named after him)

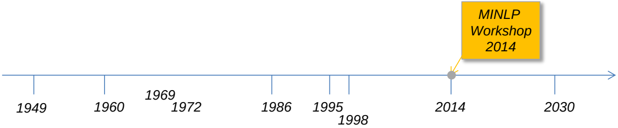
1900: Lars Ahlfors (1907-1996) (mathematics) (Fields medal in 1936)



Contents

1. Introduction – a short background to MINLP

A short background to MINLP



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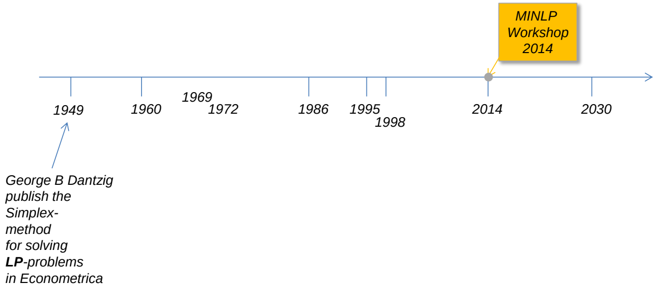
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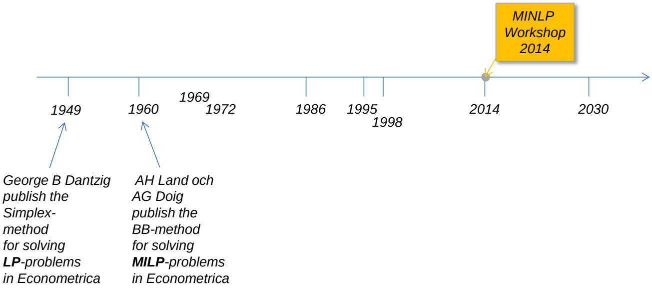
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(Typical laptop 2014: 16GB RAM & 64-bit operating system)

H-316, 16kB primary memory

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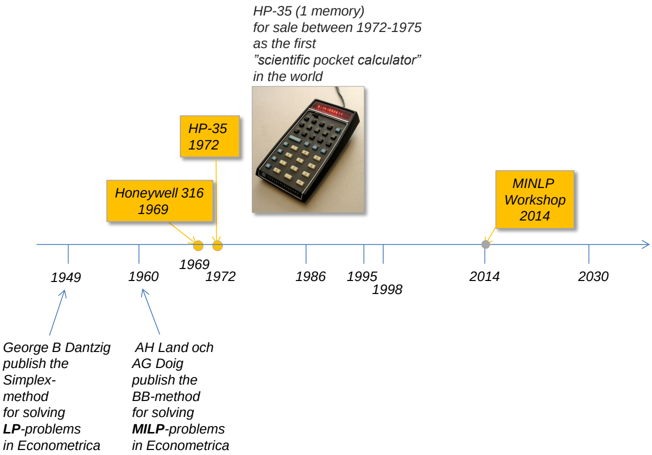
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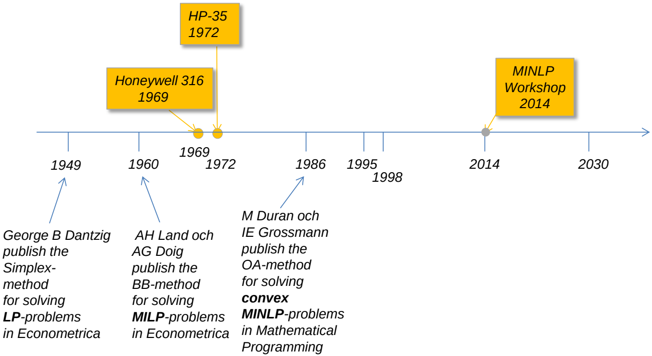
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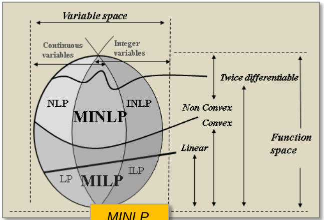

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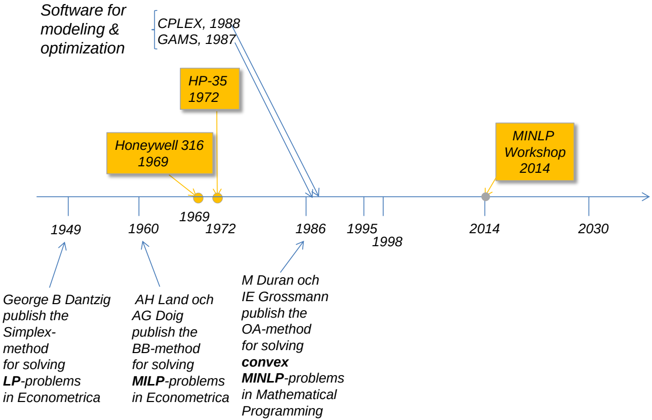
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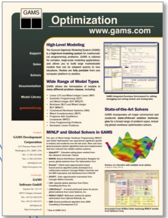

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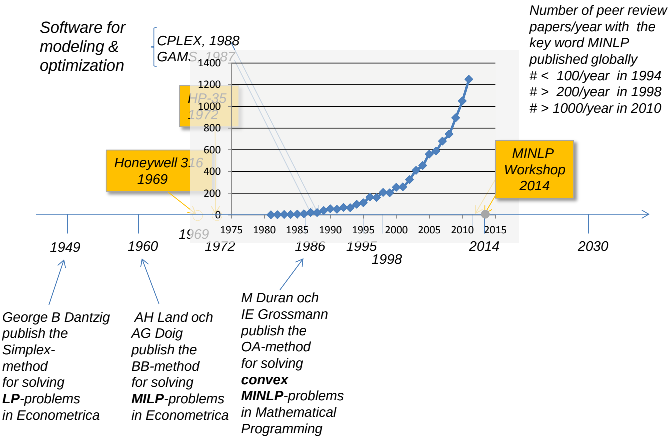
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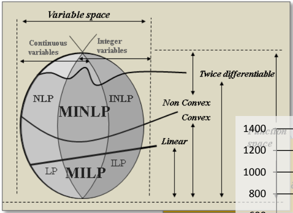

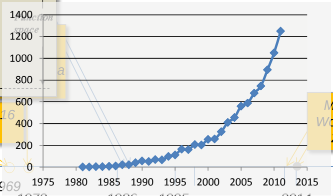

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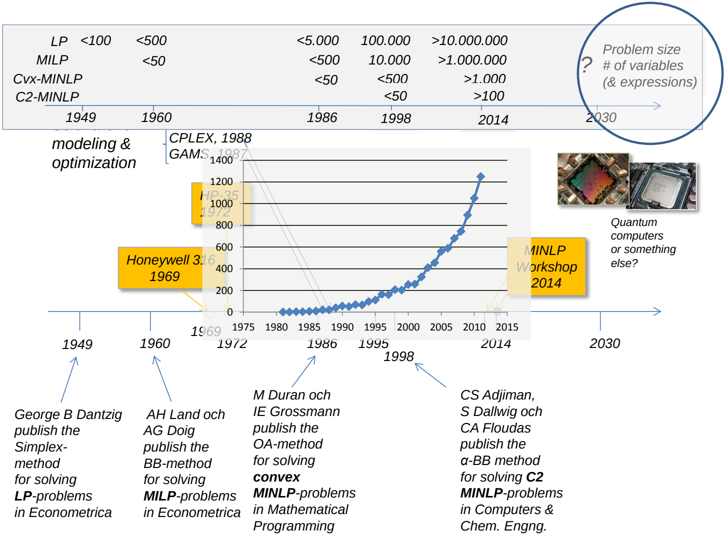

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C2-MINLP <50 >100
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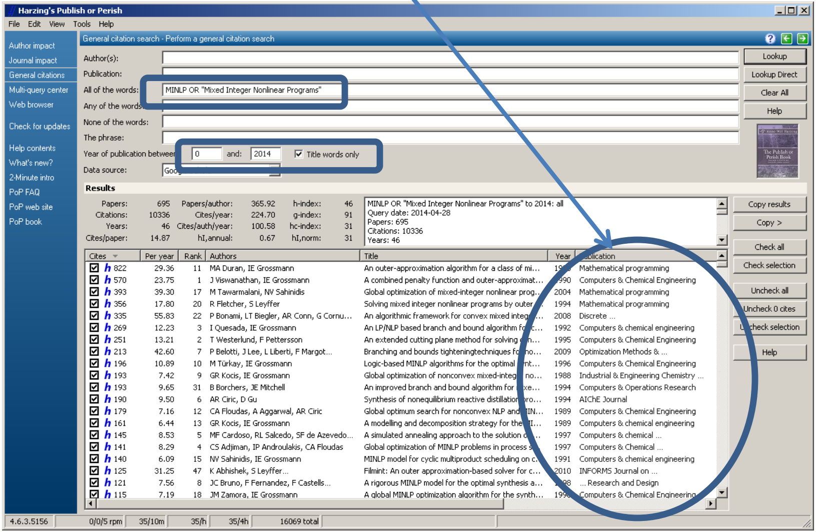
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570 23.75 1 J Viswanathan, IE Grossmann A combined penalty function and outer-approximat... Computers & Chemical Engineering
393 39.30 17 M Tawarmalani, NV Sahinidis Global optimization of mixed-integer nonlinear prog... 2004 Mathematical programming
356 17.80 20 R Fletcher, S Leyffer Solving mixed integer nonlinear programs by outer... 1994 Mathematical programming
335 55.83 22 P Bonami, LT Biegler, AR Conn, G Cornu... An algorithmic framework for convex mixed integ... 2008 Discrete ...
269 12.23 3 I Quesada, IE Grossmann An LP/NLP based branch and bound algorithm fo... 1992 Computers & chemical engineering
251 13.21 2 T Westerlund, F Pettersson An extended cutting plane method for solving... 1995 Computers & Chemical Engineering
213 42.60 7 P Belotti, J Lee, L Liberti, F Margot... Branching and bounds tighteningtechniques fo... 2009 Optimization Methods & ...
196 10.89 10 M Türkay, IE Grossmann Logic-based MINLP algorithms for the optimal... 1996 Computers & Chemical Engineering
193 7.42 9 GR Kocis, IE Grossmann Global optimization of nonconvex mixed-integ... 1988 Industrial & Engineering Chemistry ...
193 9.65 31 B Borchers, JE Mitchell An improved branch and bound algorithm for... 1994 Computers & Operations Research
190 9.50 6 AR Ciric, D Gu Synthesis of nonequilibrium reactive distillation... 1994 AIChE Journal
179 7.16 12 CA Floudas, A Aggarwal, AR Ciric Global optimum search for nonconvex NLP and... 1989 Computers & Chemical Engineering
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145 8.53 5 MF Cardoso, RL Salcedo, SF de Azevedo... A simulated annealing approach to the solution... 1997 Computers & chemical ...
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140 6.09 15 NV Sahinidis, IE Grossmann MINLP model for cyclic multiproduct scheduling on... 1991 Computers & chemical engineering
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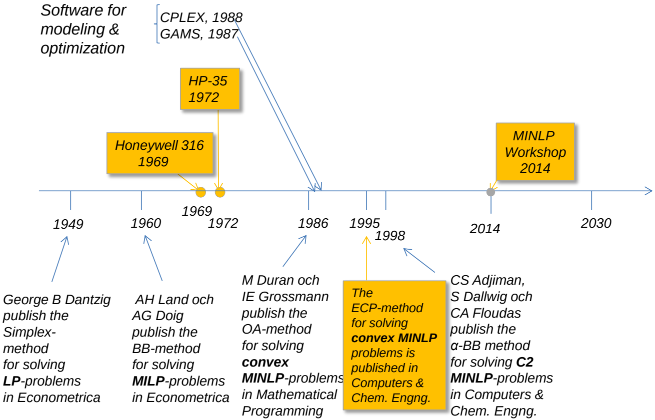
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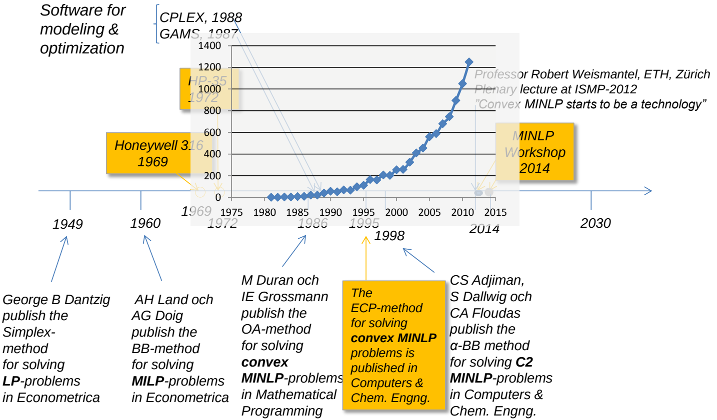
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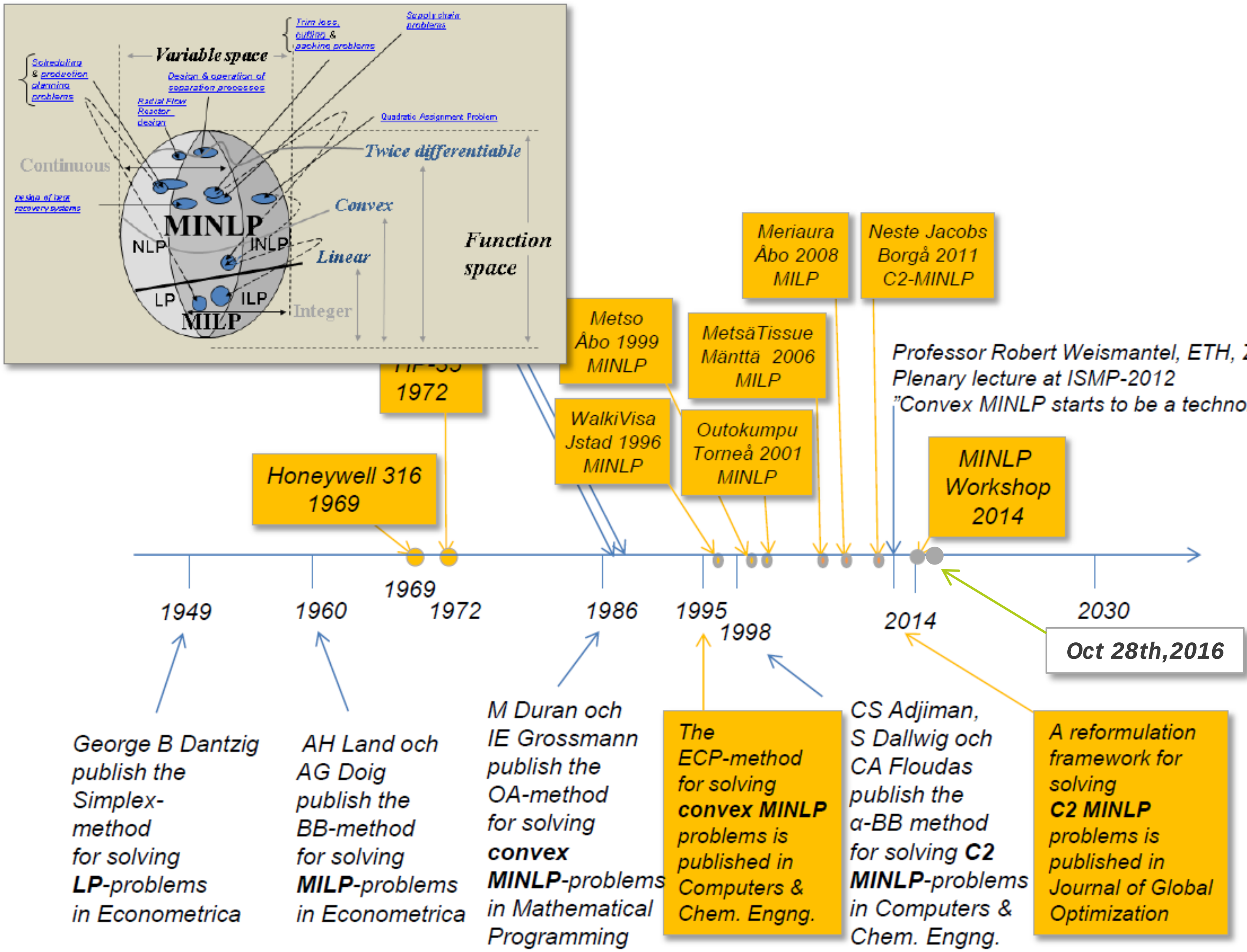
Variable space
Trim loss, cutting & packing problems
Supply chain problems
Scheduling & production planning problems
Design & operation of separation processes
Radial Flow Reactor design
Quadratic Assignment Problem
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Twice differentiable
Design of heat recovery systems
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A reformulation framework for solving **C2 MINLP** problems is published in Journal of Global Optimization

2. Aspects on algorithms for convex MINLP problems

Convex functions

Problem (P1)

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g(x) \leq 0, \end{array}$$

where f and g are convex functions.

Convex functions or convex sets

Problem (P1)

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g(x) \leq 0, \end{array}$$

where f and g are convex functions.

Problem (P2)

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C, \end{array}$$

where f is a convex function, $C = \{x | g(x) \leq 0\}$, and g are convex/quasiconvex functions.

Smooth or nonsmooth functions

- Does the convergence properties of a considered "convex MINLP" solver still hold true if the functions are not differentiable but convex/quasiconvex?

	convex	quasiconvex
smooth twice differentiable (C^2)	?	?
smooth once differentiable (C^1)	?	?
nonsmooth continuous	?	?
locally Lipschitz continuous	?	?

Nonsmooth functions in MINLP

Question: Is it possible to only replace gradients with subgradients in order to handle nonsmooth functions rigourously in algorithms for differentiable convex problems?

Answer: Not for all convex MINLP algorithms!

- Yes, *e.g.,* for ECP
- No, for certain versions of OA, *e.g.,* the linear OA[1]:

Algorithm 1 (Linear Outer Approximation).
Initialization: y^0 is given; set $i=0$, $T^{-1}=\emptyset$, $S^{-1}=\emptyset$ and $\text{UBD}=\infty$.
REPEAT
(1) Solve the subproblem $\text{NLP}(y^i)$, or the feasibility problem $\text{F}(y^i)$ if $\text{NLP}(y^i)$ is infeasible, and let the solution be x^i.
(2) Linearize the objective and (active) constraint functions about (x^i, y^i). Set $T^i=T^{i-1}\cup\{i\}$ or $S^i=S^{i-1}\cup\{i\}$ as appropriate.
(3) IF ($\text{NLP}(y^i)$ is feasible and $f^i<\text{UBD}$) THEN update current best point by setting $x^*=x^i$, $y^*=y^i$, $\text{UBD}=f^i$.
(4) Solve the current relaxation M^i of the master program M, giving a new integer assignment y^{i+1} to be tested in the algorithm. Set $i=i+1$.
UNTIL(M^i is infeasible).

[1] Fletcher, R. and Leyffer, S., Solving mixed integer nonlinear programs by outer approximation, Mathematical Programming 66, pp. 327–349, 1994.

A convex nonsmooth example where the gradient is replaced by a subgradient[2]

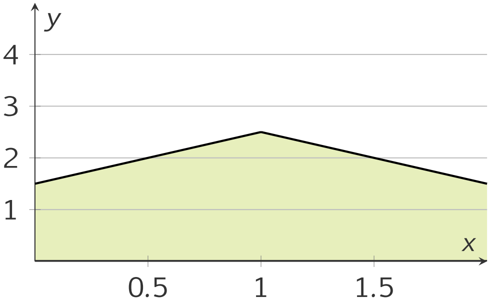
$$
\begin{array}{ll}
\text{minimize} & 2x - y \\
\text{subject to} & g(x,y) \leq 0 \\
 & y - 4x - 1 \leq 0 \\
 & 0 \leq x \leq 2, \quad y \in Y = \{0,1,2,3,4,5\},
\end{array}
\qquad (E)
$$

where

$$g(x,y) = \max\left\{-\frac{3}{2} - x + y,\ -\frac{7}{2} + y + x\right\}.$$

[2] Eronen, V.-P., Mäkelä, M. M. and Westerlund, T., On the generalization of ECP and OA methods to nonsmooth convex MINLP problems, Optimization, pp. 1–17, iFirst, available online, 2012.

Solving with the linear outer approximation



Initialization: $y^0 = 3$

Step 1: Solve the subproblem NLP(y^0) or the feasibility problem $F(y^0)$ if NLP(y^0) is infeasible, and let the solution be x^0.

- There are no feasible points in the problem NLP(y^0), thus the feasibility problem F_{y^0} will be solved:

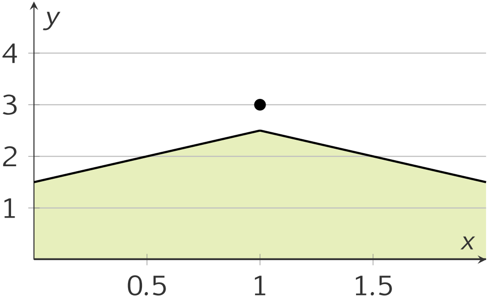
$$\begin{aligned} &\text{minimize} && \mu \\ &\text{subject to} && \max\left\{\frac{3}{2}-x,\ -\frac{1}{2}+x\right\} \leq \mu \\ &&& 2-4x \leq 0 \\ &&& 0 \leq x \leq 2. \end{aligned} \qquad (F_{y^0})$$

- The solution of F_{y^0} is $x^0 = 1$ with $\mu = 1/2$.

Step 2: Linearize g at the point $(x^0, y^0) = (1,3)$ for the next relaxed MILP master problem M^0.

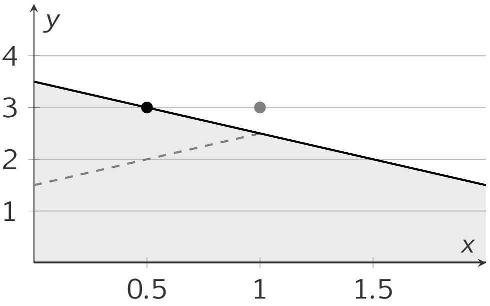
- Both the functions $-3/2 - x + y$ and $-7/2 + y + x$ have the same value $1/2$ at the point (x^0, y^0) and thus the subdifferential is

$$\partial g(1,3) = \left\{(\alpha, 1)^T | \alpha \in [-1,1]\right\}. \qquad (1)$$



- Since we may select an abitrary subgradient we may choose, *e.g.*, $\xi(x^0, y^0) = (1,1)^T$. Thus the new linear constraint is

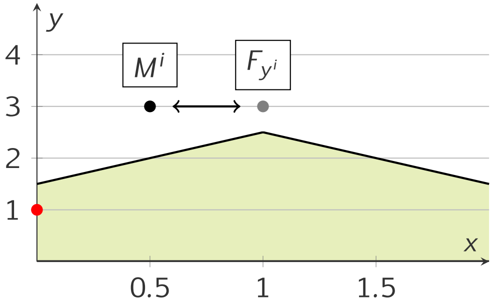
$$\frac{1}{2} + (1,1)(x-1, y-3)^T \leq 0 \quad \Rightarrow \quad x + y - \frac{7}{2} \leq 0.$$



$$
\begin{array}{ll}
\text{minimize} & 2x - y \\
\text{subject to} & x + y - 7/2 \leq 0 \\
 & y - 4x - 1 \leq 0 \\
 & 0 \leq x \leq 2, \quad y \in Y.
\end{array}
\qquad (M^0)
$$

- The solution point of (M^0) is $(1/2, 3)$. Set $i = i + 1$, $y^1 = 3$.

Repeat steps 1–4: Until M^i is infeasible.



- Hence $y^1 = y^0$ and $F_{y^1} \equiv F_{y^0}$. Thus LOA may generate an infinite loop between points $(1, 3)$ and $(1/2, 3)$.
- Both of them are infeasible but the problem (E) has a feasible point $(0, 1)$ for example, where the objective function $2x - y$ has the value -1.

3. A new algorithm for solving convex MINLP problems

- A new interior point based algorithm for solving convex MINLP problems to global optimality is introduced.
- Roots:
  - Kelley's cutting plane algorithm 1960[3]
  - The extended cutting plane (ECP) algorithm 1995[4]
- Cutting planes are replaced with supporting hyperplanes using a line search procedure.
- An interior point is required for the line search.

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[3] Kelley, Jr., J., The cutting-plane method for solving convex programs, Journal of the SIAM, vol. 8(4), pp. 703–712, 1960.

[4] Westerlund, T. and Pettersson, F., An extended cutting plane method for solving convex MINLP problems, Computers & Chemical Engineering 19, pp. 131–136, 1995.

An example

$$
\begin{aligned}
\text{minimize} \quad & c^T x = -x_1 - x_2 \\
\text{subject to} \quad & 1/x_1 + 1/x2 - x_1^{0.5} x_2^{0.5} + 4 \le 0 \\
& 0.15(x_1 - 8)^2 + 0.1(x_2 - 6)^2 + 0.025 e^{x_1} x_2^{-3} - 5 \le 0 \\
& 2x_1 - 3x_2 - 2 \le 0 \\
& 1 \le x_1 \le 20, \quad 1 \le x_2 \le 20, \quad x_1 \in \mathbb{R}, \quad x_2 \in \mathbb{Z}.
\end{aligned}
$$

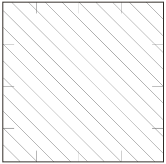
THE MINLP PROBLEM SCOPE

The ESH algorithm solves convex MINLP problems of the type

$$\text{find } x^* \in \underset{x \in C \cap L \cap Y}{\arg\min}\, c^T x \tag{P}$$

where $x = [x_1, x_2, \ldots, x_N]^T$ belongs to the compact set

$$X = \{x \mid \underline{x}_i \leq x_i \leq \bar{x}_i,\ i = 1, \ldots, N\} \subset \mathbb{R}^n,$$



the feasible region is defined by $C \cap L \cap Y$

$$\begin{aligned} C &= \{x \mid g_m(x) \leq 0,\ m = 1, \ldots, M,\ x \in X\} \\ L &= \{x \mid Ax \leq a,\ Bx = b,\ x \in X\} \\ Y &= \{x \mid x_i \in \mathbb{Z},\ i \in I_{\mathbb{Z}},\ x \in X\} \end{aligned}$$

and C is a convex set.

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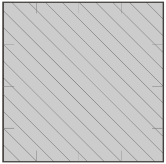

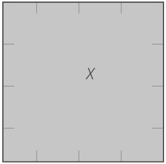

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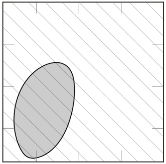

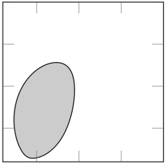

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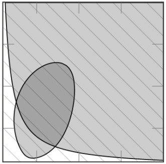

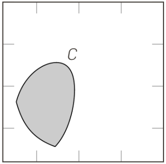

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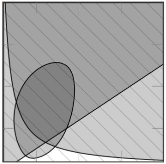

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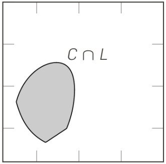

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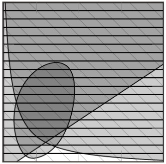

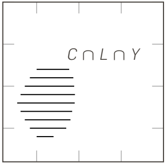

BREAKDOWN OF THE ESH ALGORITHM

Interior point search step

Obtain a feasible, relaxed interior point (satisfying C) by solving a NLP problem.

LP step (optional)

Solve simple LP problems (initially in $X \cap L$) to obtain an initial overestimating linear set.

MILP step

Solve MILP problems to find the optimal solution to (P).

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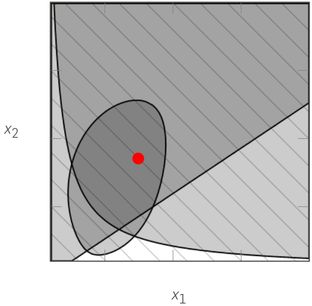
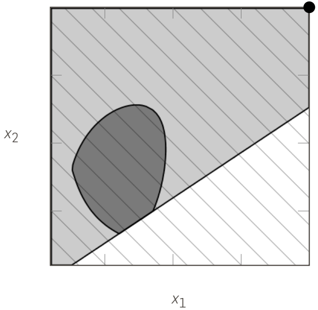
INTERIOR POINT SEARCH



If an interior point is not given, obtain a feasible, relaxed interior point (satisfying all the nonlinear constraints in C) by solving a NLP problem.

LP STEP (OPTIONAL)



Solve simple LP problems and conduct a line search procedure to obtain supporting hyperplanes giving a first linear relaxation of the convex set C.

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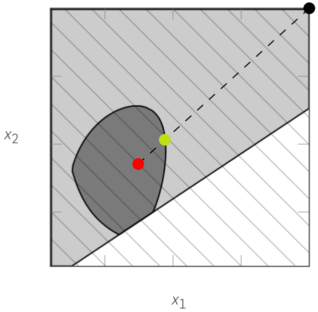

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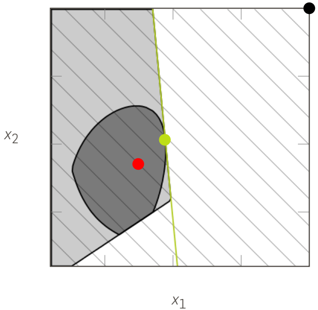

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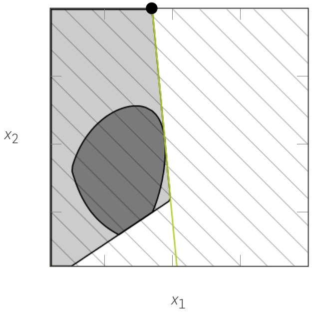

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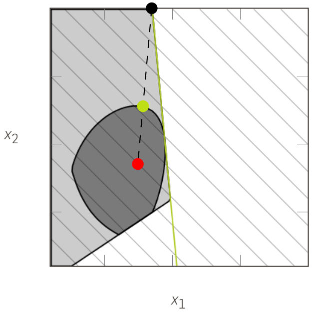

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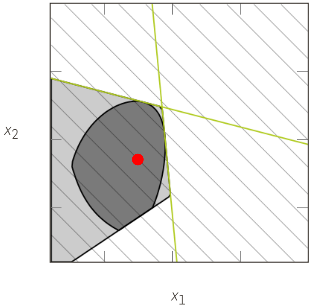

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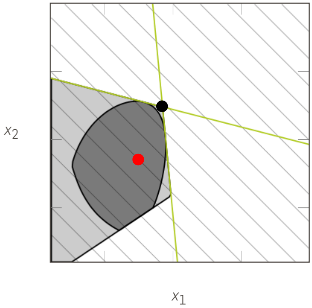

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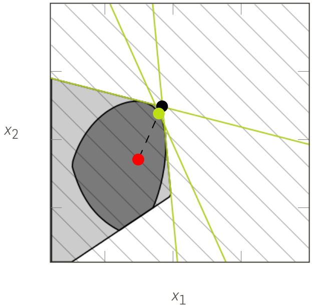

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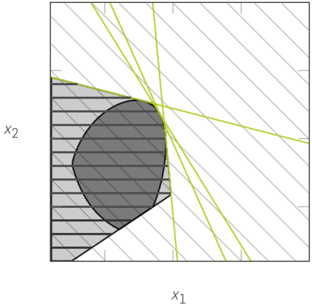

Finally include the integer requirements and solve MILP problems using a corresponding procedure to find the optimal solution to (P).

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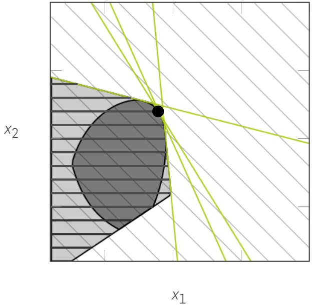

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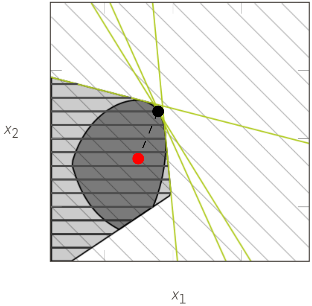

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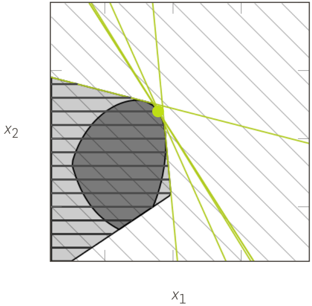

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QUADRATIC AND NONLINEAR OBJECTIVE FUNCTIONS

Normally, a nonlinear objective function $f(x)$ is rewritten as a constraint

$$f(x) - \mu \leq 0$$

and the new objective is to minimize the auxiliary variable μ.

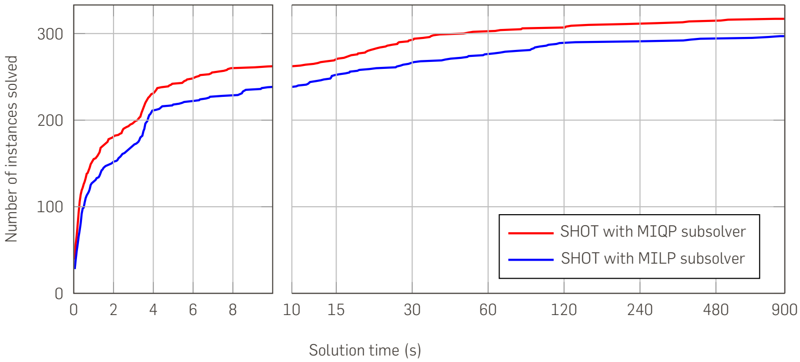
Many MILP solvers can directly solve MIQP problems:

- Then $f(x) = x^T Q x + c^T x$, where Q positive semidefinite.
- Gives the exact objective instead of a linearization.

Quadratic constraints can also be handled by some solvers.

- Numerical issues may lead to trouble with proving semidefiniteness.
- Not always more effective than using the ESH algorithm for these constraints.

IMPACT OF USING THE QUADRATIC OBJECTIVE STRATEGY



A performance profile of the number of problem instances solved by SHOT to an objective duality gap $\leq 1\%$ with a MIQP or MILP subsolver.

SOLUTION LIMIT STRATEGY

It is possible to set the number of feasible solutions to find before terminating the MILP/MIQP subsolver.

Can be used to speed up the initial MILP iterations:

» Optimal solution of intermediate subproblems not required.

» Reduces solution time significantly in many cases.

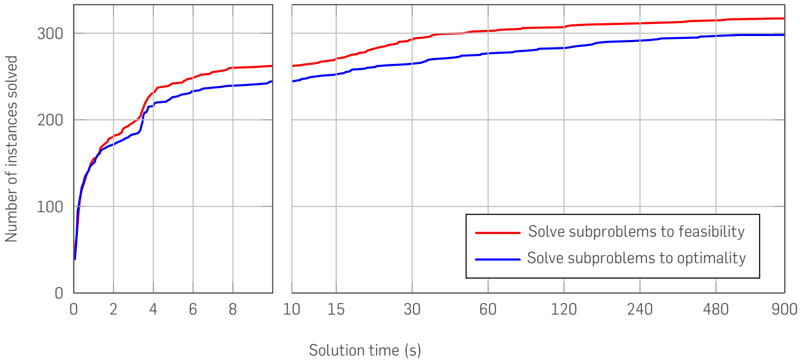
» If no constraints are added to the subproblem, the solution limit can be increased without rebuilding the branching tree.

Solution limit strategy *

1. Initially set SOLLIM $= 1$.
2. Solve MILP/MIQP subproblem and obtain solution x.
3. Terminate if x is MILP optimal and ESH termination criterion fulfilled.
4. Increase SOLLIM and goto step 2 if x is MILP optimal and $\max_m g_m(x) \leq \epsilon_{SL}$.
5. Add supporting hyperplanes and goto step 2.

* Westerlund T. and Pörn R. (2002). Solving Pseudo-Convex Mixed Integer Optimization Problems by Cutting Plane Techniques. *Optimization and Engineering*, 3, 253-280.

SOLUTION LIMIT STRATEGY IMPACT



Performance profiles of the number of problem instances solved by SHOT to an objective duality gap $\leq 1\%$ with or without an increasing solution limit strategy.

BENCHMARKS AGAINST OTHER SOLVERS

The following MINLP solvers available in GAMS 24.4.1 were used:

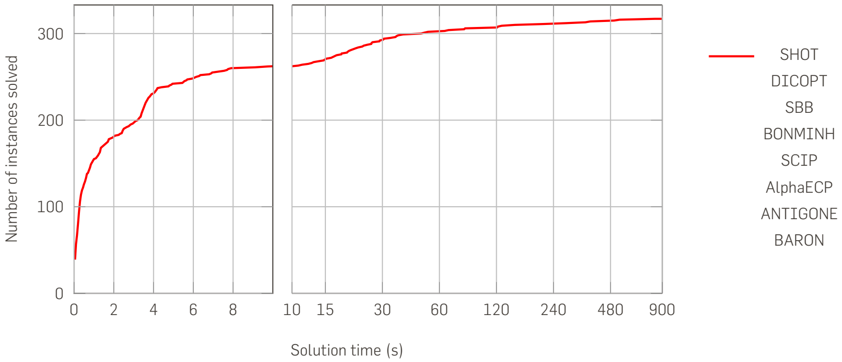
» AlphaECP (with convex strategy)
» ANTIGONE
» BARON
» BONMINH (with recommended convex strategy, B-Hyb)
» DICOPT
» SBB
» SCIP (with convex strategy)

CPLEX and CONOPT were used as subsolvers and the time limit per problem was 900 s.

The same problem set as before was used, *i.e.*, all 333 convex MINLP problems in MINLPLib 2.

The total computational time for all solvers was about 150 h.

PERFORMANCE PROFILE



A performance profile of the number of problem instances solved to an objective duality gap $\leq 1\%$.

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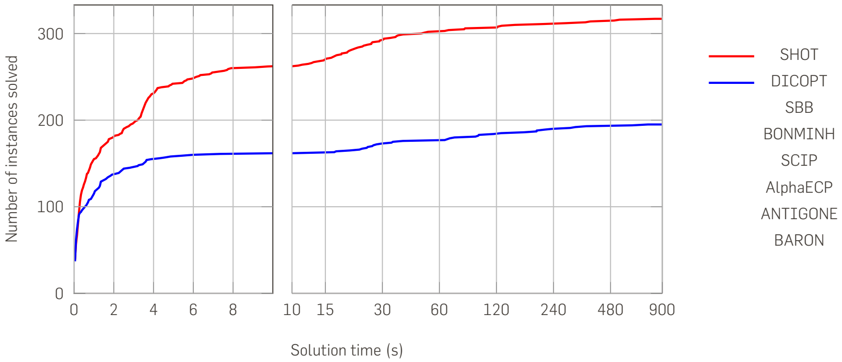

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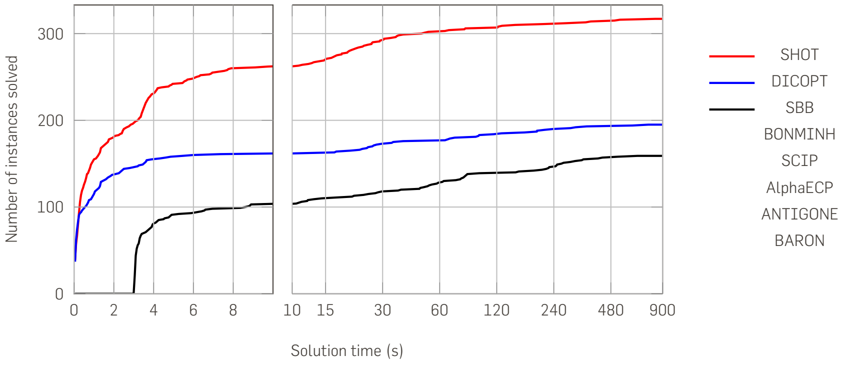

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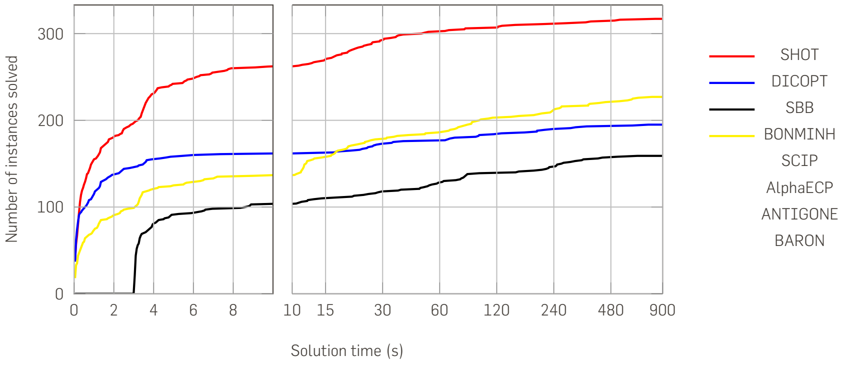

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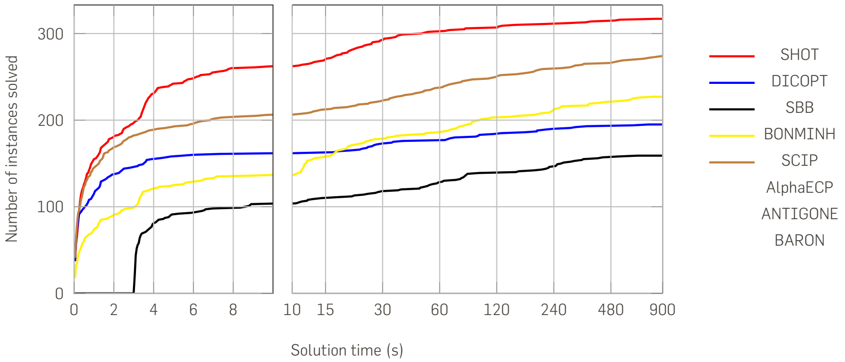

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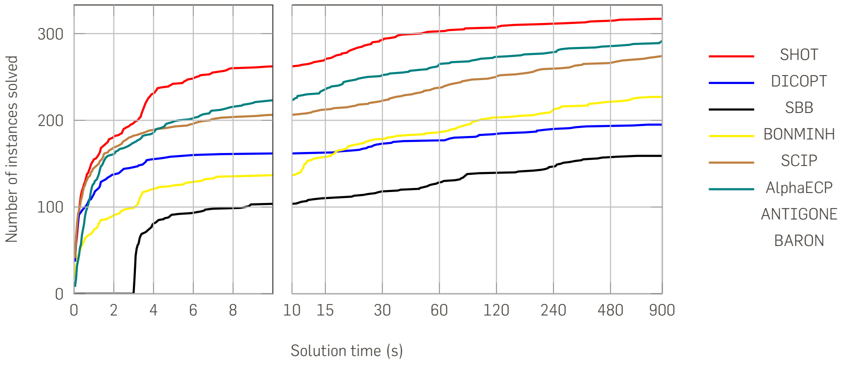

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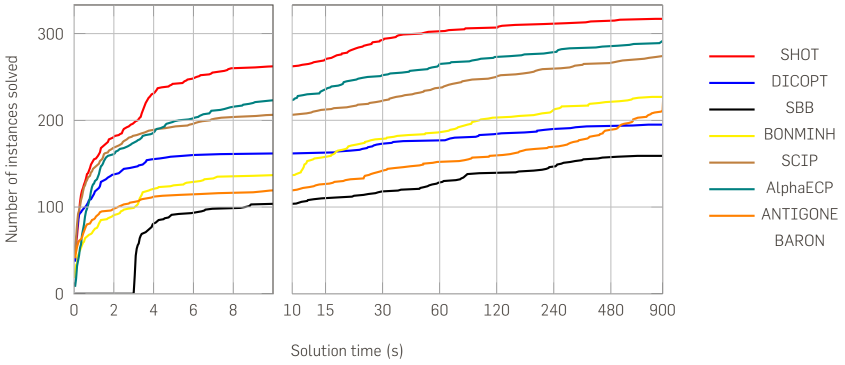

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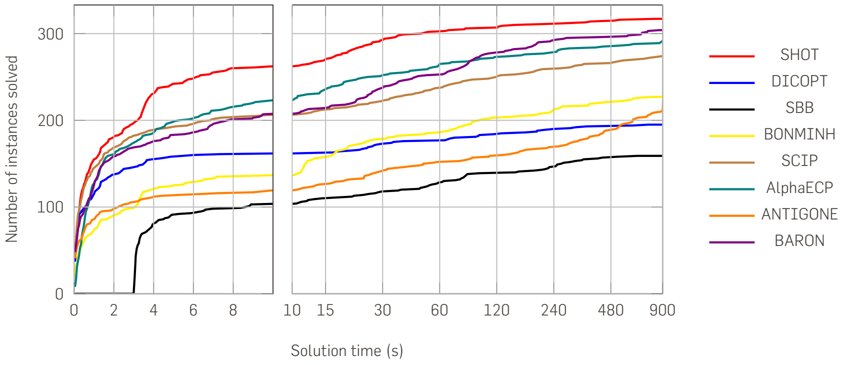

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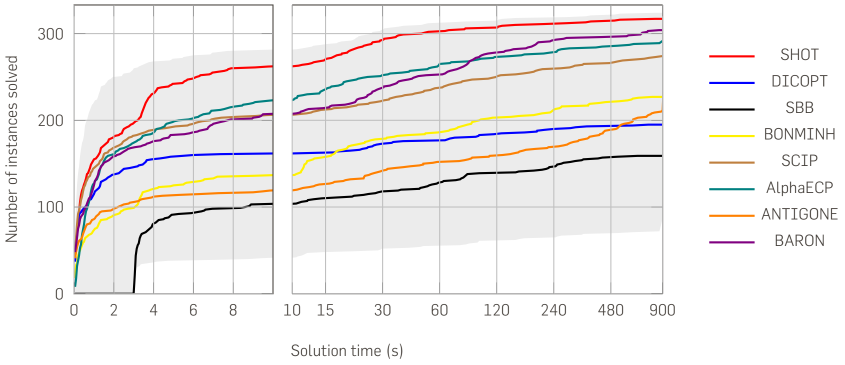

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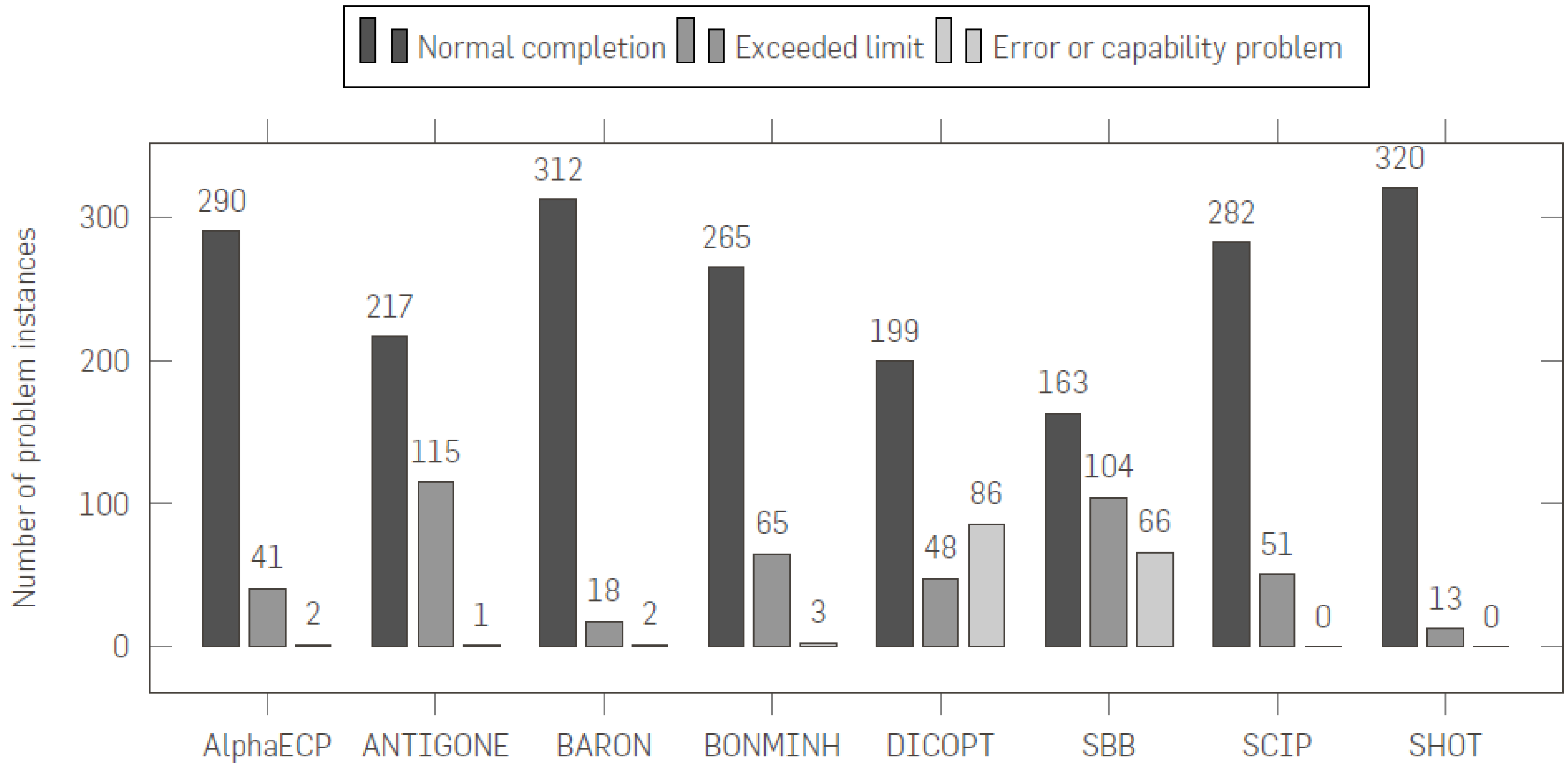
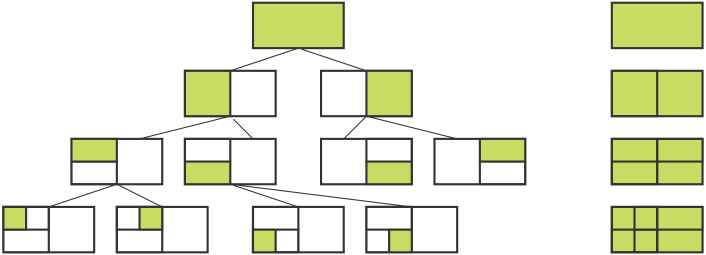
REASONS FOR TERMINATION



The termination statuses for the solvers as provided by PAVER 2. Note that a the solution can be optimal even though a limit (*e.g.*, time) has been reached, the solver has simply not proven optimality.

4. Aspects on frameworks for nonconvex MINLP problems

Convex relaxation: branching vs reformulation



- **Branching:** n convex subproblems (the subproblems with the green domains are solved using a branching strategy)
- **Reformulation:** the entire nonconvex MINLP problem is reformulated to a convex relaxed MINLP problem solved sequentially.

Convex envelopes of functions or sets
for tight convex relaxations

- Does a convex envelope $c(x) = \text{conv}\, g(x)$ of a nonconvex function g in an inequality constraint $g(x) \leq 0$ give the tightest convex relaxation of $g(x) \leq 0$ when replacing it with $c(x) \leq 0$?

Convex relaxations and envelopes in literature

Tuy 1998

"A nonconvex inequality constraint $g(\mathbf{x}) \leq 0$, $\mathbf{x} \in X$, where X is a convex set in $\mathbb{R}^n$, can often be handled by replacing it with a convex inequality constraint $c(\mathbf{x}) \leq 0$ where $c(\mathbf{x})$ is a convex minorant of $g(\mathbf{x})$ on X. The latter inequality is then called a convex relaxation of the former. **Of course, the tightest relaxation is obtained when $c(\mathbf{x}) = \text{conv } g(\mathbf{x})$, the convex envelope, *i.e.,* the largest convex minorant, of $g(\mathbf{x})$.**"

Let's see...

- Could it be possible to find some function q, other than $c(x) = \operatorname{conv} g(x)$, with the property:

$$N \subset C_q \subset C_c,$$

where

$$\begin{aligned} N &= \{x | g(x) \leq 0\} \\ C_q &= \{x | q(x) \leq 0\} \\ C_c &= \{x | c(x) \leq 0\} \end{aligned}$$

for all $x \in X$ such that C_q would still be a convex set?

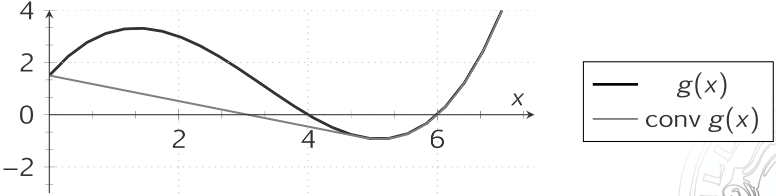
The convex envelope of a function

Consider the function

$$g(x) = 0.00506x^4 + 0.09553x^3 - 1.2774x^2 + 2.8821x + 1.5.$$

The convex envelope of the nonconvex function $g(x)$ on the interval $[0, 7]$ is given by

$$\text{conv } g(x) = \begin{cases} -0.488764x + 1.5 & \text{if } 0 \leq x \leq 4.8312, \\ g(x) & \text{if } 4.8312 < x \leq 7. \end{cases}$$



The αBB underestimator, Floudas (2000)

Convex underestimator for twice-differentiable functions

A function $g(\mathbf{x}) \in C^2$ has the convex underestimator

$$\boxed{\hat{g}(\mathbf{x}) = g(\mathbf{x}) + \sum_i \alpha(\underline{x}_i - x_i)(\overline{x}_i - x_i)}$$

for $x_i \in [\underline{x}_i, \overline{x}_i]\ \forall i$ if and only if the parameter α fulfills

$$\alpha \geq \max\left\{0, -\tfrac{1}{2}\min_i \lambda_i\right\}$$

where the λ_i's are the eigenvalues of the Hessian of $g(\mathbf{x})$ on the interval $[\underline{x}_i, \overline{x}_i]$.
Different methods for calculating the α-values are available, *e.g.*, the scaled Gerschgorin method.

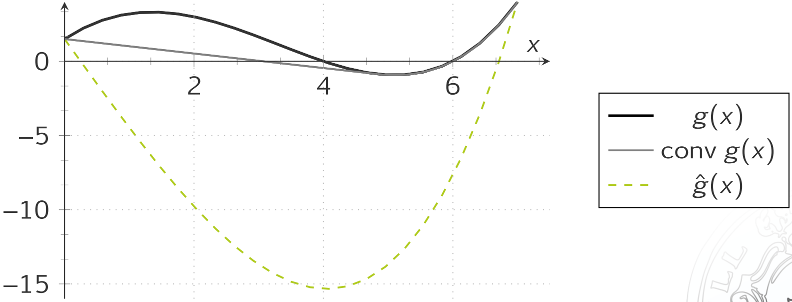
The αBB underestimator, illustration

- For example for the function

$$g(x) = 0.00506x^4 + 0.09553x^3 - 1.2774x^2 + 2.8821x + 1.5,$$

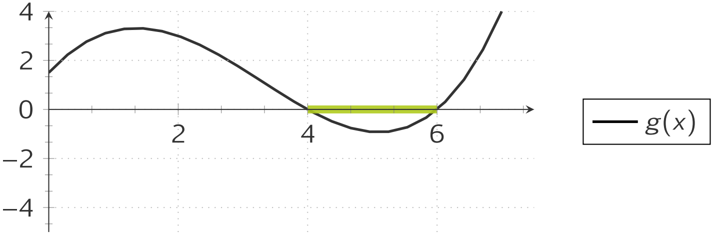
where $0 \leq x \leq 7$, the αBB underestimator becomes

$$\hat{g}(x) = g(x) + 1.2774(0 - x)(7 - x).$$



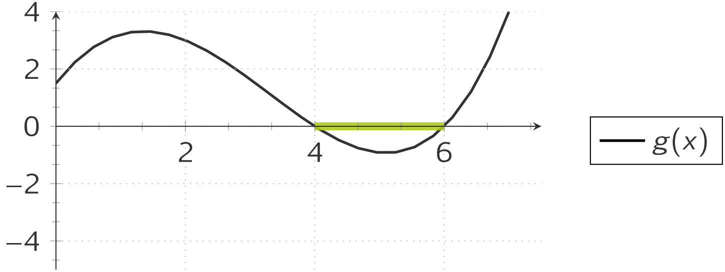
Convex envelope of the level set

- Observe that the convex envelope of a function $g(x)$ is the tightest convex relaxation of the function in question, but does not generally give the tightest convex relaxation of a level set $L = \{x \mid g(x) \leq \alpha\}$ (in this case $\alpha = 0$).



- The tightest convex relaxation of L is conv L, *i.e.,* the convex hull of L.
- The convex envelope of the set L is given by the border of its convex hull.

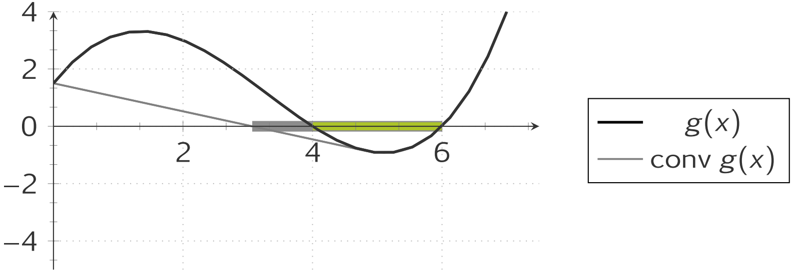
Convex relaxations of the level set $L = \{x | g(x) \leq 0\}$



- The level sets $L_\alpha^g = \{x | g(x) \leq \alpha\}$ are:

$$L_{\alpha=0}^g = [4, 6]$$

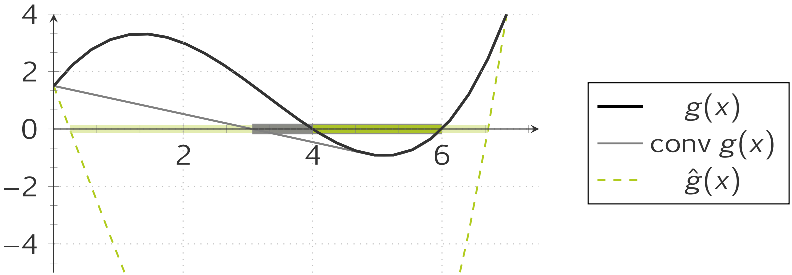
Convex relaxations of the level set $L = \{x | g(x) \leq 0\}$



- The level sets $L_\alpha^g = \{x | g(x) \leq \alpha\}$ are:

$$L_{\alpha=0}^{g} = [4, 6] \qquad L_{\alpha=0}^{\text{conv } g} = [3.069, 6]$$

Convex relaxations of the level set $L = \{x | g(x) \leq 0\}$

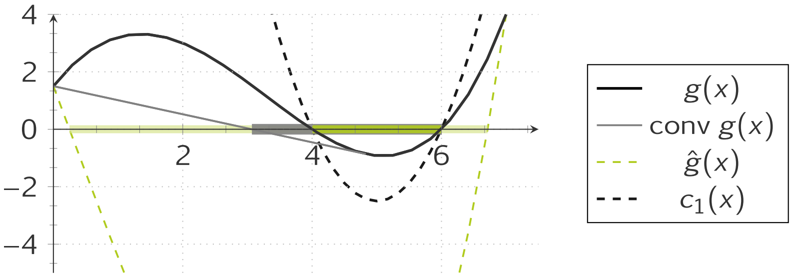


- The level sets $L_{\alpha}^{g} = \{x | g(x) \leq \alpha\}$ are:

$$L_{\alpha=0}^{g} = [4,6] \qquad L_{\alpha=0}^{\mathrm{conv}\, g} = [3.069,6]$$

$$L_{\alpha=0}^{\hat{g}} = [0.248,6.713]$$

Convex relaxations of the level set $L = \{x|g(x) \leq 0\}$

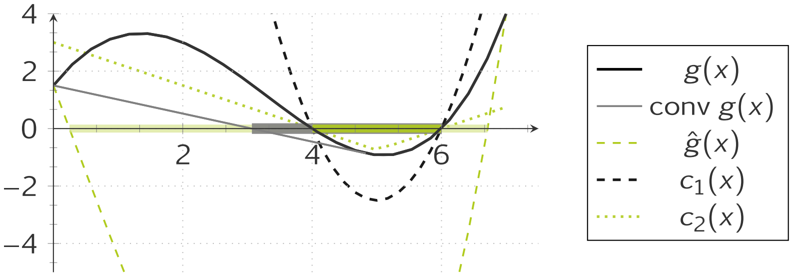


- The level sets $L^g_\alpha = \{x|g(x) \leq \alpha\}$ are:

$$L^g_{\alpha=0} = [4,6] \qquad L^{\text{conv } g}_{\alpha=0} = [3.069,6]$$
$$L^{\hat{g}}_{\alpha=0} = [0.248,6.713] \qquad L^{c_1}_{\alpha=0} = [4,6]$$

- A possible tight convex relaxation: $c_1(x) = \frac{5}{2}(x-4)(x-6)$.

Convex relaxations of the level set $L = \{x | g(x) \leq 0\}$



- The level sets $L_\alpha^g = \{x | g(x) \leq \alpha\}$ are:

$$L_{\alpha=0}^{g} = [4, 6] \qquad L_{\alpha=0}^{\mathrm{conv}\, g} = [3.069, 6]$$

$$L_{\alpha=0}^{\hat{g}} = [0.248, 6.713] \qquad L_{\alpha=0}^{c_1} = L_{\alpha=0}^{c_2} = [4, 6]$$

- Another tight convex relaxation:
  $c_2(x) = \max\left\{-\frac{3}{4}(x-4),\ \frac{3}{4}(x-6)\right\}$.

A nonconvex size constraint in two dimensions

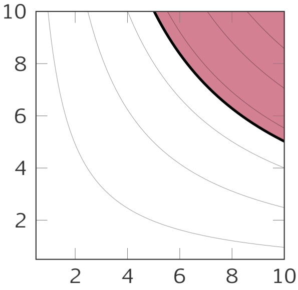
- Consider the inequality constraint

$$g(\mathrm{x}) \leq 0,$$

where

$$g(\mathrm{x}) = 50 - x_1 \cdot x_2, \quad 0.5 \leq x_1,\ x_2 \leq 10.$$

- The contour plot of the constraint function g is



McCormick convex relaxation

- The convex envelope of the negative bilinear term $-x_1 x_2$ is

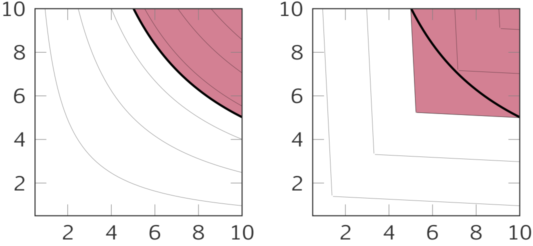
$$\max\{-\overline{x}_1 x_2 - \underline{x}_2 x_1 + \overline{x}_1 \underline{x}_2,\ -\underline{x}_1 x_2 - \overline{x}_2 x_1 + \underline{x}_1 \overline{x}_2\}$$

  where the bounds of the variables are $\underline{x}_i \leq x_i \leq \overline{x}_i$.

- If $0.5 \leq x_1,\ x_2 \leq 10$, we then obtain

$$\begin{aligned} \text{conv}\, g(\mathbf{x}) = 50 - \max\{&-10 \cdot x_1 - 0.5 \cdot x_2 + 5, \\ &-0.5 \cdot x_1 - 10 \cdot x_2 + 5\} \end{aligned}$$

The level sets for the McCormick relaxation



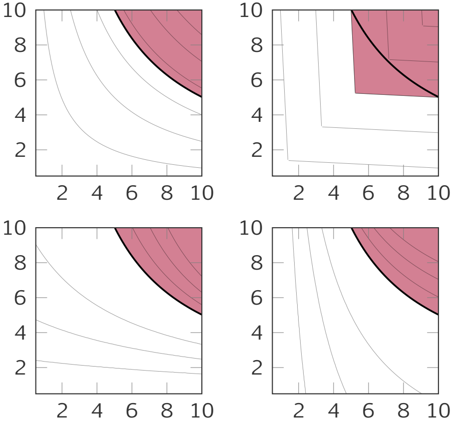
Left: The level set $L^{g}_{\alpha=0}$. *Right:* The level set $L^{\text{conv } g}_{\alpha=0}$.

- Observe that, although $L^{g}_{\alpha=0}$ is a convex set, replacing $g(\mathbf{x}) \leq 0$ with conv $g(\mathbf{x}) \leq 0$ does not give the tightest convex relaxation of $L^{g}_{\alpha=0}$.

A convex reformulation

- By reformulating
$$g(\mathbf{x}) = 50 - x_1 \cdot x_2$$
at $g(\mathbf{x}) = 0$ we can, in this case, obtain the following convex constraints exactly defining the border of the level set $L^{g}_{\alpha=0}$:
$$c_1(\mathbf{x}) = \frac{50}{x_2} - x_1 \qquad \text{and} \qquad c_2(\mathbf{x}) = \frac{50}{x_1} - x_2.$$
- Since $c_1(\mathbf{x})$ and $c_2(\mathbf{x})$ exactly define the border of $L^{g}_{\alpha=0}$, it follows that
$$L^{c_1}_{\alpha=0} \equiv L^{c_2}_{\alpha=0} \equiv L^{g}_{\alpha=0}.$$

The level sets for the convex reformulation



Upper left: The level set $L^{g}_{\alpha=0}$. *Upper right:* The level set $L^{\operatorname{conv} g}_{\alpha=0}$.
Lower left: The level set $L^{c_1}_{\alpha=0}$. *Lower right:* The level set $L^{c_2}_{\alpha=0}$.

3D illustration of the relaxations

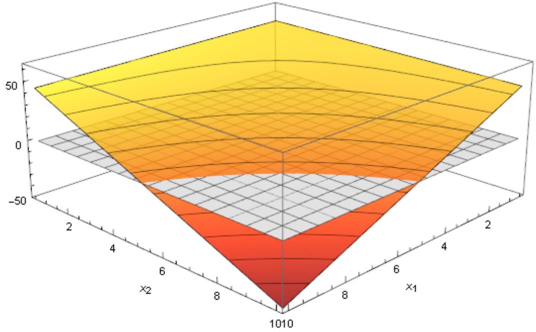


Illustration of $g(x)$

3D illustration of the relaxations

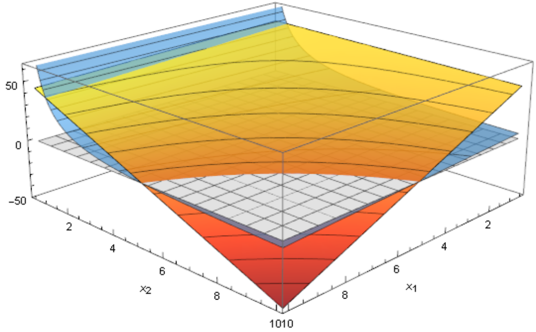


Illustration of $g(\mathrm{x})$ and $c_1(\mathrm{x})$

3D illustration of the relaxations

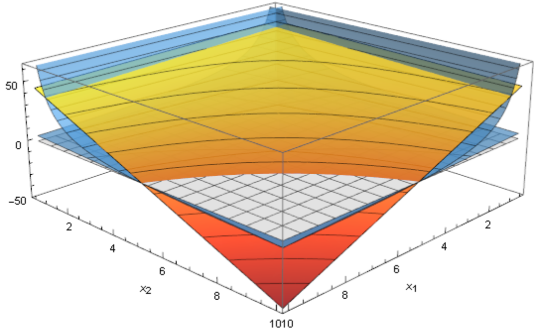


Illustration of $g(\mathbf{x})$, $c_1(\mathbf{x})$ and $c_2(\mathbf{x})$

5. A reformulation algorithm for solving C^2 MINLP problems

Introduction

- A framework for reformulating nonconvex (twice-differentiable – C^2) mixed integer nonlinear programming (MINLP) problems to convex form is presented.
  - The framework is an extension to a previously introduced reformulation technique for signomial problems.
  - For C^2-constraints, convex reformulations are made in an extended variable-space using variants of the αBB quadratic convex underestimator.
  - With the framework, a nonconvex problem can be reformulated to a larger convex MINLP problem solved in one step or to a sequence of smaller relaxed MINLP problems solved iteratively.

The considered problem-type

Nonconvex problem

$$\begin{aligned} \text{min.} \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & \mathbf{q}(\mathbf{x}) + \mathbf{h}(\mathbf{x}) \leq 0 \\ & \underline{\mathbf{x}} \leq \mathbf{x} \leq \overline{\mathbf{x}} \end{aligned}$$

- $f(\mathbf{x})$ is a convex function
- $\mathbf{q}(\mathbf{x})$ are convex functions
- $\mathbf{h}(\mathbf{x})$ are nonconvex twice-differentiable (C^2) functions
- the variables in $\mathbf{x}$ are reals, binaries or integers

- Nonconvex twice-differentiable functions (incl. signomials) can be convexified using an αBB-type reformulation.

$$\hat{h}(x) = h(\mathbf{x}) + \sum_{i=1}^{N} \left(\alpha_i x_i^2 - \widehat{W}_i \right) \leq 0, \quad \mathbf{x} = (x_1, x_2, \ldots, x_N)$$

where the Hessian of $\hat{h}(x)$ will be:

$$\hat{H} = H + 2\,diag\,(\alpha_i)$$

and the α_i values obtained i.e. by Gerschgorin's circle theorem

Gerschgorin's circle theorem

Theorem

Let $A \in \mathbb{C}^{n\times n}$ with entries a_{ij} and define $R_i = \sum_{j\neq i} |a_{ij}|$. Every eigenvalue of A lies within at least one of the Gerschgorin disks

$$D(a_{ii}, R_i) = \{x : |x - a_{ii}| \leq R_i\}.$$

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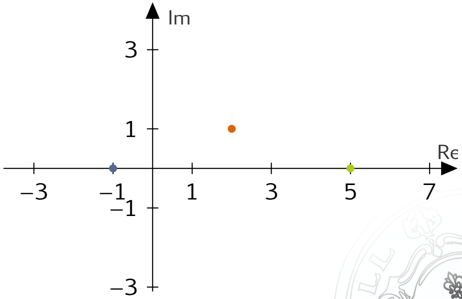
Example

$$A = \begin{bmatrix} 2+i & 2 & -1 \\ 1 & 5 & i \\ 1 & -1 & -1 \end{bmatrix}$$



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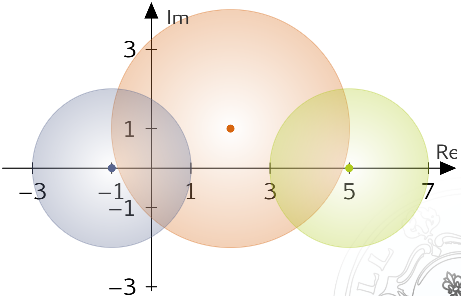

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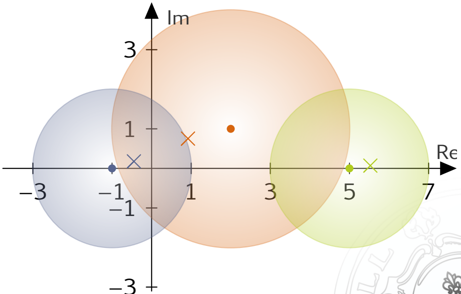
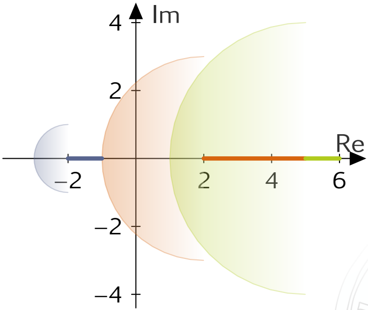


Extending Gerschgorin's circle theorem to interval matrices

- The circle theorem can be extended to interval matrices by considering the worst case.
- Positive-semidefiniteness is wanted, therefore "worst case" should be interpreted as lowest eigenvalue.

Example

$$H = \begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}$$



Diagonal αBB using the Gerschgorin Method

- The function is underestimated by adding the perturbation

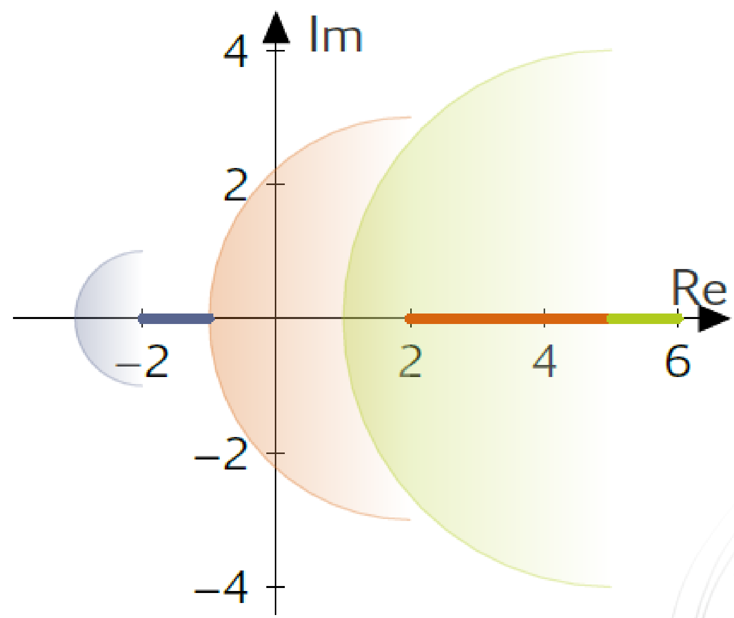
$$\hat{h}(x) = h(\mathbf{x}) + \sum_{i=1}^{N} \left(\alpha_i x_i^2 - \widehat{W}_i \right) \leq 0, \quad \mathbf{x} = (x_1, x_2, \ldots, x_N)$$

- To guarantee positive-semidefiniteness we set the constraints $\underline{h_{ii}} - R_i + 2\alpha_i \geq 0,\ i = 1, 2, \ldots, n.$

$$\begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}$$

$$+ \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$= \begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}$$



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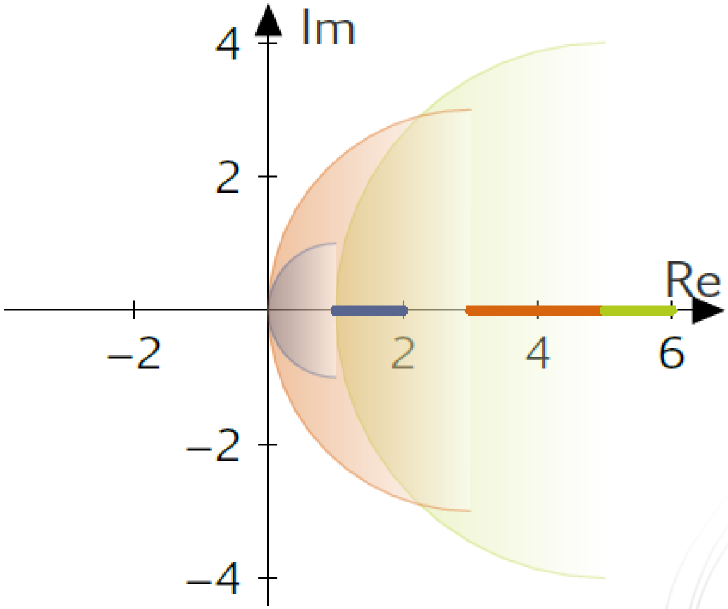
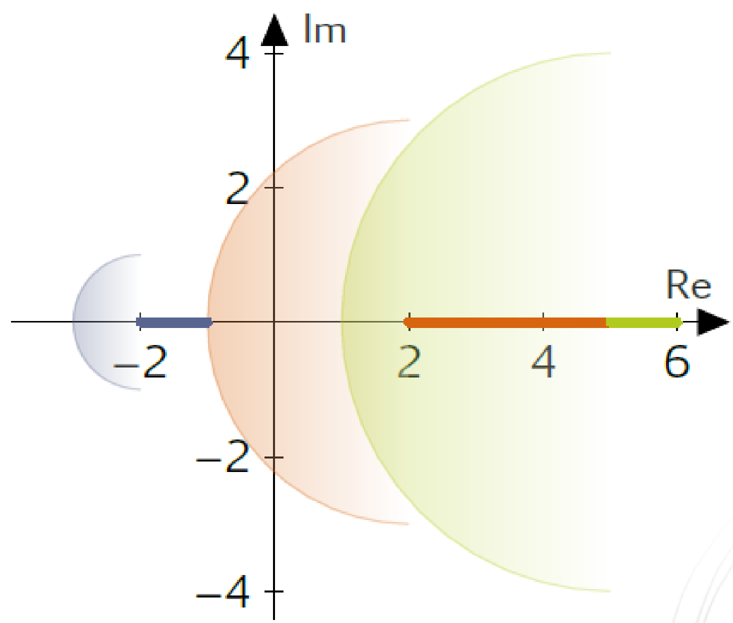
$$\begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix} + \begin{bmatrix} 1 & & \\ & 0 & \\ & & 3 \end{bmatrix} = \begin{bmatrix} [3,6] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [1,4] \end{bmatrix}$$



Diagonal and off-diagonal αBB

- The function can also be underestimated by adding $\hat{h}(x) = h(x) + \sum_{i=1}^{N} \left(\alpha_i x_i^2 - \widehat{W}_i \right) + \sum_i \sum_{j>i} \beta_{ij} x_i x_j$ as in Skjäl et al. (2012).
- To guarantee positive-semidefiniteness we can then manipulate the diagonal and off-diagonal elements of the resulting Hessian matrix: the radius and midpoint of each Gerschgorin circle will be altered in the constraints $\underline{h_{ii}} + 2\alpha_i - \sum_{j \neq i} \left| h_{ij}^{'} + \beta_{ij} \right| \geq 0 \; \forall i,\; h_{ij}^{'} \in [\underline{h_{ij}}, \overline{h_{ij}}]$.

$$
\begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}
+ \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
= \begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}
$$



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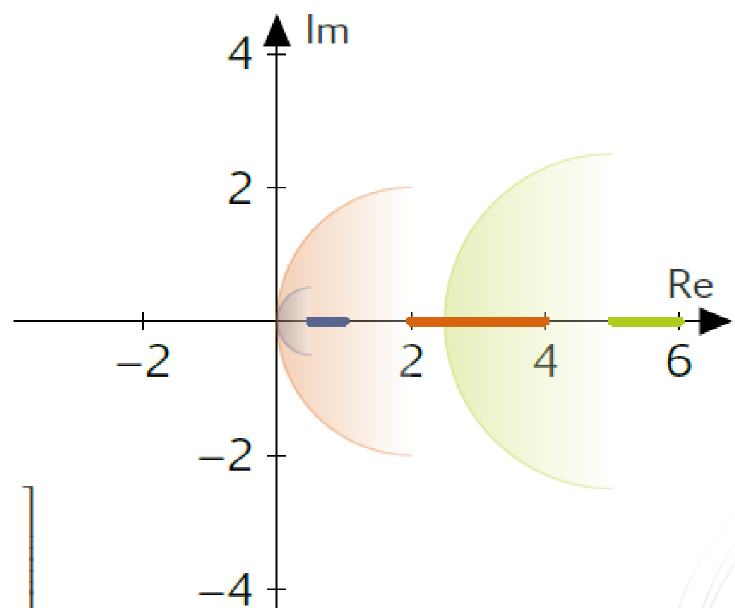
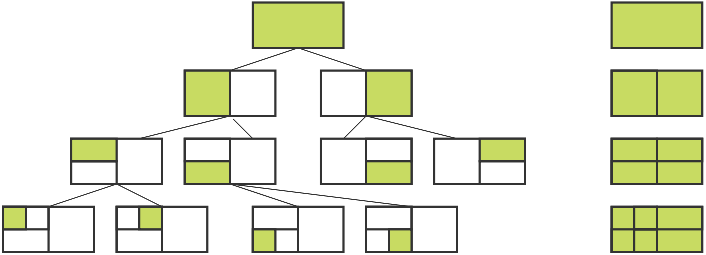
$$\begin{bmatrix} [2,5] & [-1,3] & 0 \\ [-1,3] & [5,6] & [-1,0] \\ 0 & [-1,0] & [-2,-1] \end{bmatrix}$$

$$+\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 1/2 \\ 0 & 1/2 & 5/2 \end{bmatrix}$$

$$= \begin{bmatrix} [2,5] & [-2,2] & 0 \\ [-2,2] & [5,6] & [-1/2,1/2] \\ 0 & [-1/2,1/2] & [1/2,3/2] \end{bmatrix}$$



Branching vs reformulation



- **Branching:** n convex subproblems (the subproblems with the green domains are solved using a branching strategy)
- **Reformulation:** a sequence of convex MINLP problems are solved (the whole domain is considered in each iteration)

Including αBB in the reformulation framework

- To be able to reformulate the problem in subdomains without branching, a convex quadratic function αx^2 is added to and a variable $\widehat{W}$ subtracted from the nonconvex C^2 constraint, *i.e.*,

$$\underbrace{h(x) + \alpha x^2 - \widehat{W}}_{\text{convex}} \leq 0.$$

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- If α is large enough, then the reformulated constraint will be convex.

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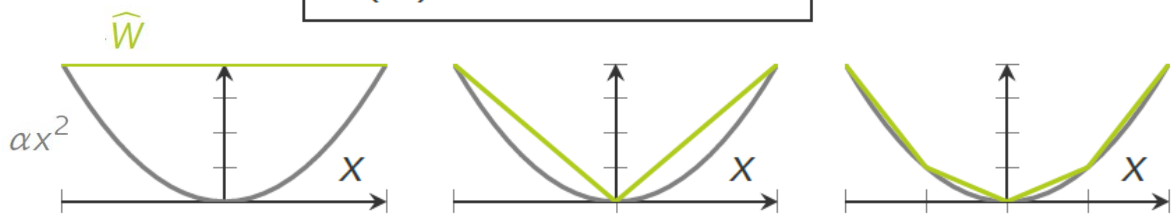
$$\underbrace{h(x) + \alpha x^2 - \widehat{W}}_{\text{convex}} \leq 0.$$

- If α is large enough, then the reformulated constraint will be convex.
- If $\alpha x^2 - \widehat{W} \leq 0$, then the reformulated constraint underestimates the original one.

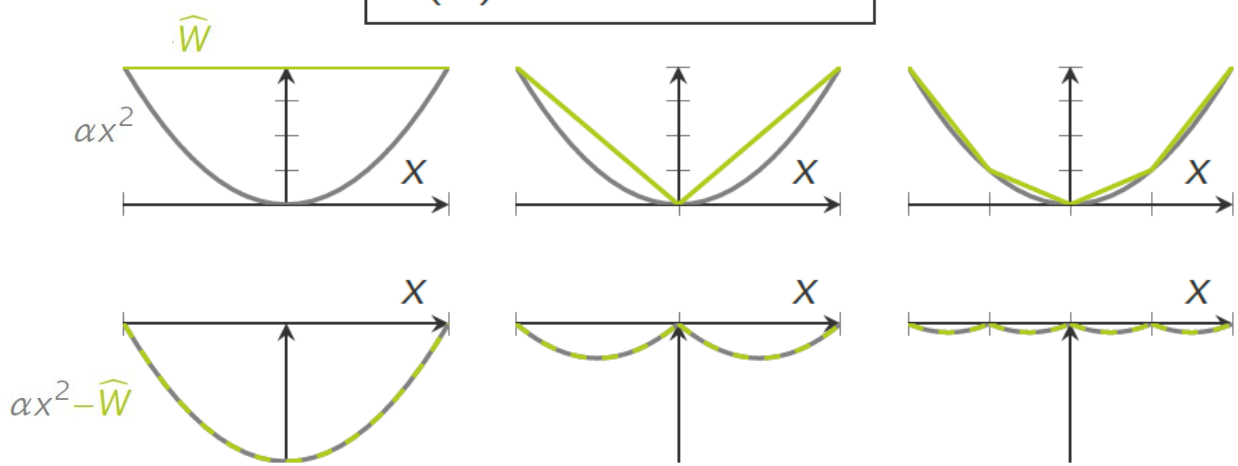
The convex reformulation in subdomains

$$\boxed{h(x) + \alpha x^2 - \widehat{W} \leq 0}$$



The convex reformulation in subdomains

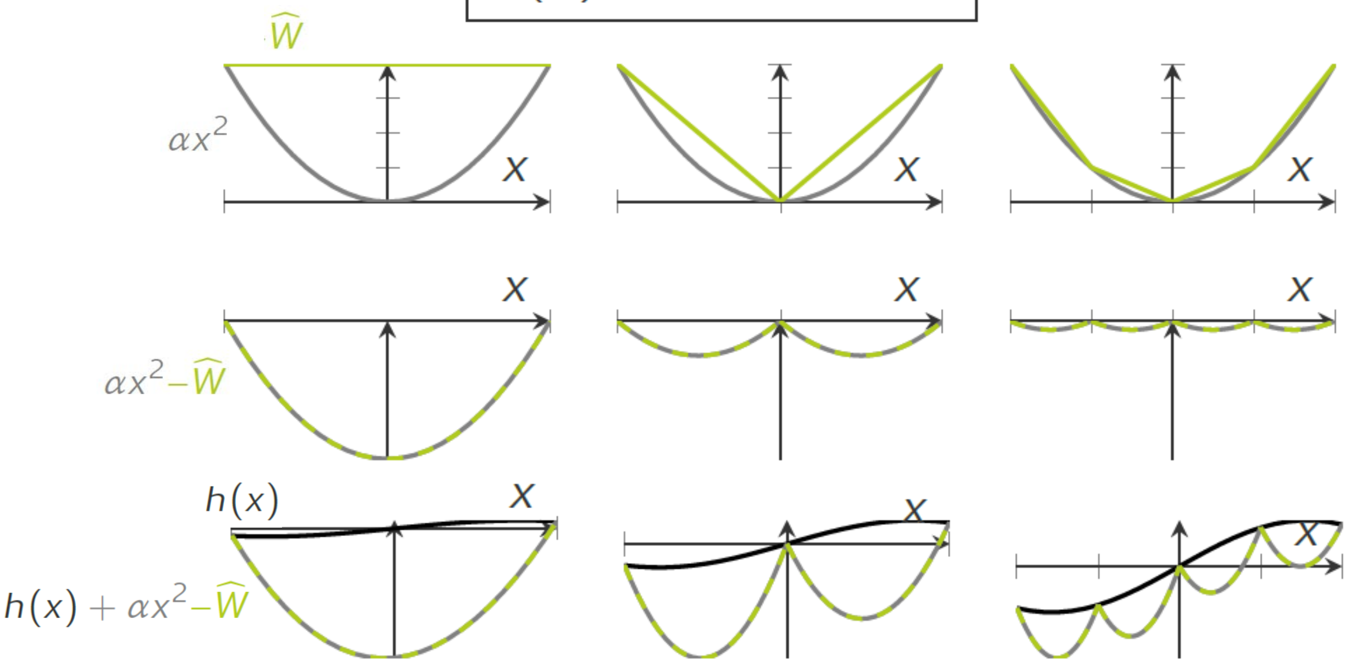
$$\boxed{h(x) + \alpha x^2 - \widehat{W} \leq 0}$$



- If α in αx^2 is large enough then $h(x) + \alpha x^2 - \widehat{W}$ will be convex.
- If $\widehat{W}$ is given by a PLF of αx^2 then $h(x)$ is also underestimated in each subdomain since $\alpha x^2 - \widehat{W} \leq 0$.

The convex reformulation in subdomains

$$\boxed{h(x) + \alpha x^2 - \widehat{W} \leq 0}$$

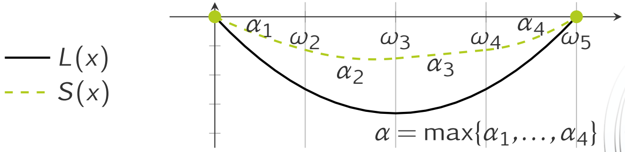


The spline αBB underestimator

- The spline αBB-underestimator is a smooth convex piecewise polynomial expression

$$S(x) = \begin{cases} \alpha_1 x^2 + \beta_1 x + \gamma_1 & \text{if } x \in [\omega_1, \omega_2] \\ \alpha_2 x^2 + \beta_2 x + \gamma_2 & \text{if } x \in [\omega_2, \omega_3] \\ \vdots & \vdots \\ \alpha_{K-1} x^2 + \beta_{K-1} x + \gamma_{K-1} & \text{if } x \in [\omega_{K-1}, \omega_K], \end{cases}$$

- The α_k's ensure convexity. The β_k and γ_k for $k \in \{2, \ldots, K-1\}$ ensure smoothness and continuity, and β_1, γ_1 gives $S(\omega_1) = S(\omega_K) = 0$.



Generalization to N dimensions

- The formulation can easily be extended from one to N dimensions by using the underestimators

$$h(\mathbf{x})+\sum_{i=1}^{N}\left(\alpha_i x_i^2-\widehat{W}_i\right)\leq 0,\quad \mathbf{x}=(x_1,x_2,\dots,x_N),\quad \text{or}$$

$$h(\mathbf{x})+\sum_{i=1}^{N}\left(S_i(x_i)-\widehat{S}_i\right)\leq 0,\quad \mathbf{x}=(x_1,x_2,\dots,x_N).$$

when using the reformulated versions of the original αBB and spline αBB underestimators respectively.

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$$h(\mathbf{x}) + \sum_{i=1}^{N} \left(\alpha_i x_i^2 - \widehat{W}_i \right) \leq 0, \quad \mathbf{x} = (x_1, x_2, \ldots, x_N), \quad \text{or}$$

$$h(\mathbf{x}) + \sum_{i=1}^{N} \left(S_i(x_i) - \widehat{S}_i \right) \leq 0, \quad \mathbf{x} = (x_1, x_2, \ldots, x_N).$$

  when using the reformulated versions of the original αBB and spline αBB underestimators respectively.

- Here $\widehat{W}_i$ is the PLF of $W_i = \alpha_i x_i^2$ and $\widehat{S}_i$ is the PLF of S_i.

Reformulation or implementation in a global optimization algorithm

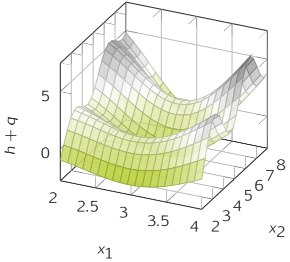
- The underestimator can be used for reformulation or directly implemented in a global optimization algorithm, *e.g.,* αGO, for solving nonconvex MINLP problems with C^2-constraints, *c.f.,* Lundell et al. (2013).
- A sequence of overestimated convex MINLP problems is solved (see Eronen et al. (2012) for convex MINLP methods) until the solution fulfills the constraints in the original nonconvex problem.
- The feasible region of the overestimated convexified problem is reduced in each iteration by improving the PLFs of $W = \alpha_i x_i^2$ or $S(x)$.

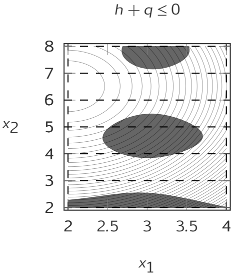
The original nonconvex MINLP problem

$$\begin{aligned} &\text{minimize} && f(x_1,x_2) = (2x_1-4)^2 + (x_2 - 13/2)^2 \\ &\text{subject to} && \underbrace{x_1\cos^2 x_2 + x_2 \sin^2 x_1 - 3/x_2}_{h(x_1,x_2)} + \underbrace{x_1/2 - 5/2}_{q(x_1)} \le 0, \\ & && 2 \le x_1 \le 4, \quad 2 \le x_2 \le 8, \quad x_1 \in \mathbb{R}, \quad x_2 \in \mathbb{Z}. \end{aligned}$$

The original nonconvex MINLP problem

$$
\begin{aligned}
\text{minimize} \quad & f(x_1, x_2) = (2x_1 - 4)^2 + (x_2 - 13/2)^2 \\
\text{subject to} \quad & \underbrace{x_1 \cos^2 x_2 + x_2 \sin^2 x_1 - 3/x_2}_{h(x_1,x_2)} + \underbrace{x_1/2 - 5/2}_{q(x_1)} \leq 0, \\
& 2 \leq x_1 \leq 4, \quad 2 \leq x_2 \leq 8, \quad x_1 \in \mathbb{R}, \quad x_2 \in \mathbb{Z}.
\end{aligned}
$$



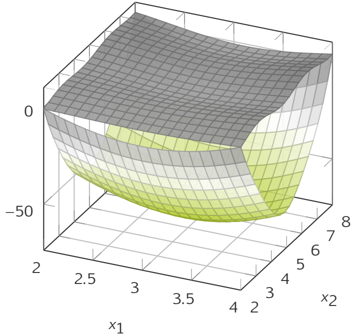


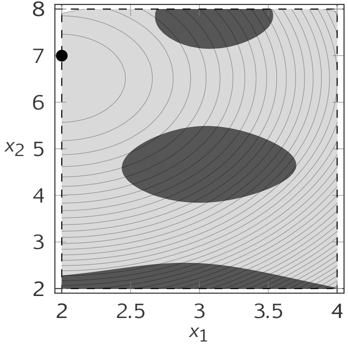
The reformulated MINLP problem

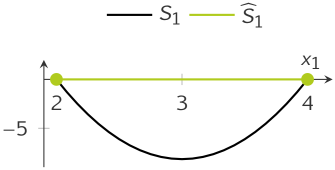
$$
\begin{aligned}
\text{minimize} \quad & f(x_1, x_2) = (2x_1 - 4)^2 + (x_2 - 13/2)^2 \\
\text{subject to} \quad & x_1 \cos^2 x_2 + x_2 \sin^2 x_1 - 3/x_2 + x_1/2 - 5/2 \\
& \qquad\qquad + S_1(x_1) + S_2(x_2) - \widehat{S}_1 - \widehat{S}_2 \le 0, \\
& \widehat{S}_1 = \mathrm{PLF}(S_1(x_2), V_1;\, \Omega_1),\ \widehat{S}_2 = \mathrm{PLF}(S_2(x_2), V_2;\, \Omega_2), \\
& 2 \le x_1 \le 4, \quad 2 \le x_2 \le 8, \quad x_1 \in \mathbb{R}, \quad x_2 \in \mathbb{Z}, \\
& V_i \text{ and } \Omega_i \text{ are sets including the variables} \\
& \text{and breakpoints in } \mathrm{PLF}_i \text{ of } S_i(x_1)
\end{aligned}
$$

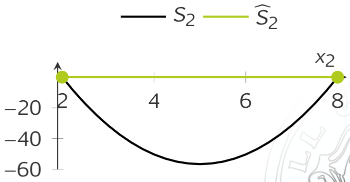
- This reformulated problem is convex in the extended variable space consisting of the original variables x_1 and x_2, as well as, those needed for the PLFs in V_1 and V_2.

αGO iteration 1

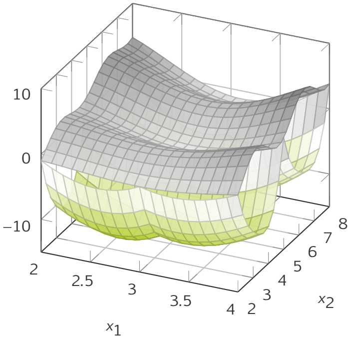


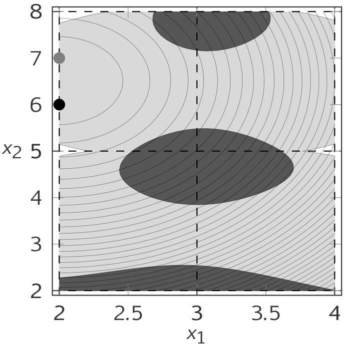


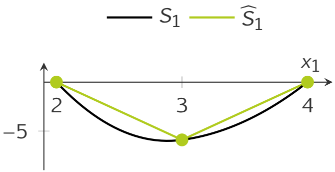


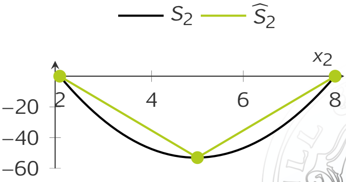


αGO iteration 2

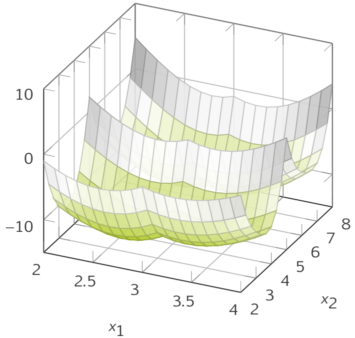


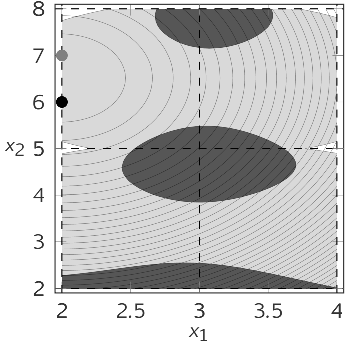


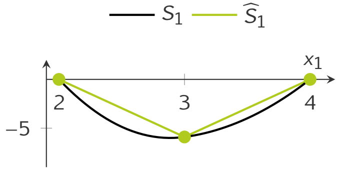


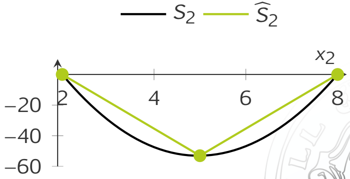


αGO iteration 2

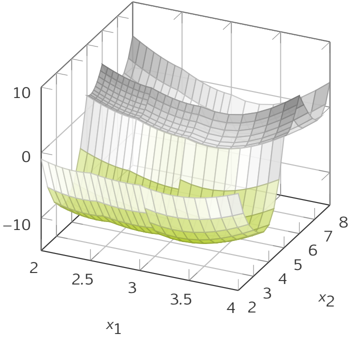


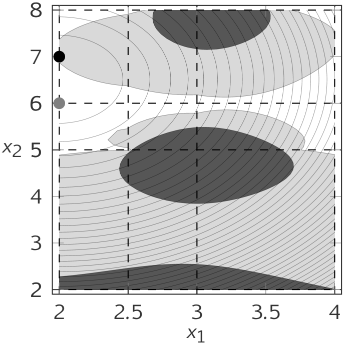


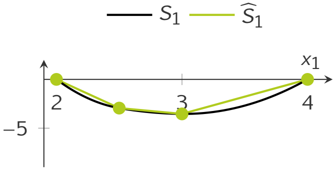


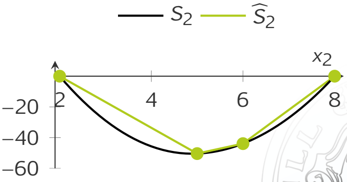


αGO iteration 3

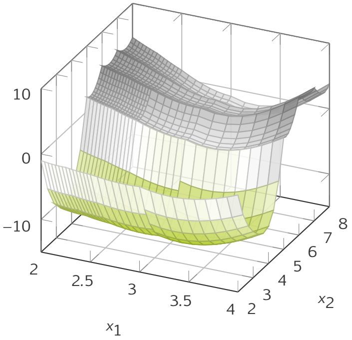


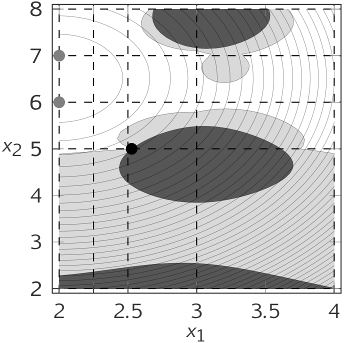


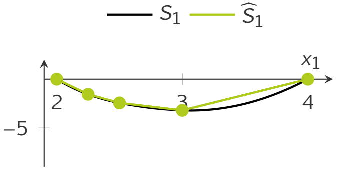


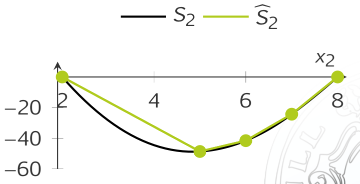


αGO iteration 4

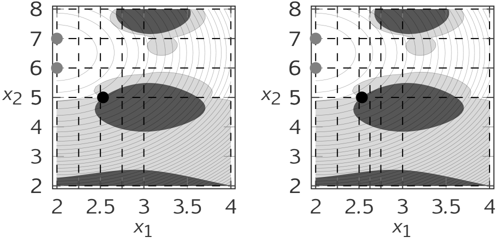








αGO iteration 5 and 6



Iter.	Regions	$f(x_1,x_2)$	x_1	x_2	$h(x_1,x_2)+q(x_1)$
1	1	0.2500	2.0	7	4.9959
2	4	0.2500	2.0	6	4.9959
3	9	0.2500	2.0	7	4.9959
4	16	3.3630	2.52749	5	0.0273
5	20	3.3767	2.53074	5	0.0139
6	24	3.3848	2.53263	5	0.0061

Summary

1. Introduction – a short background to MINLP

2. Some aspects on convex MINLP algorithms
    - Convex functions and convex sets
    - Smooth and nonsmooth functions

3. A new algorithm for solving convex MINLP problems

4. Aspects on solving nonconvex MINLP problems
    - Convex relaxations in BB and relaxation frameworks
    - Convex envelopes of functions or level sets

5. A reformulation algorithm for solving C^2 MINLP problems

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The end of the presentation

Thank you for listening!

The presentation including relevant references will be available at **www.abo.fi/ose**