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A reformulation framework for global optimization

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Main topics of the talk

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- The framework is an extension to that used in the signomial global optimization algorithm.
- Convex reformulations in an extended variable space using variants of the αBB quadratic convex underestimator.

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  - The convex relaxation is made tighter by iteratively including more breakpoints in the PLFs.
- The goal is to extend the problem scope to also include twice-differentiable functions.

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- The algorithm proposed here is based on the SGO algorithm together with quadratic convex underestimators for nonconvex C^2-functions
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- The signomial functions can be handled as either signomials or C^2-functions or using a mixture of the strategies.
- The result is a method able to solve nonconvex MINLP problems containing twice-differentiable functions to global optimality.

The considered class of MINLP problems

$$\begin{array}{lll} \text{minimize} & f(\mathbf{x}) & \mathbf{x} = (x_1, x_2, \ldots, x_N) \\ \text{subject to} & \mathbf{A}\mathbf{x} = \mathbf{a} \quad \mathbf{B}\mathbf{x} \leq \mathbf{b} & \\ & g_n(\mathbf{x}) \leq 0 & n = 1, 2, \ldots, J_n \\ & \underbrace{q_m(\mathbf{x})}_{\text{convex}} + \underbrace{\sigma_m(\mathbf{x})}_{\text{signomial}} + \underbrace{h_m(\mathbf{x})}_{\text{nonconvex}} \leq 0 & m = 1, 2, \ldots, J_m \end{array}$$

- The vector $\mathbf{x}$ can contain both continuous and integer-valued variables.
- The differentiable real functions f and g are (pseudo)convex, and the functions q, σ and h are convex, signomial and twice-differentiable (C^2) nonconvex respectively.
- A signomial function is of the form

$$\sigma(\mathbf{x}) = \sum_j c_j \prod_i x_i^{p_{ji}}.$$

Convex underestimation of C^2-functions

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Theorem

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

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

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

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

where the λ_i*'s are the eigenvalues of the Hessian matrix of* $g(\mathbf{x})$ *on the interval* $[\underline{x}_i, \overline{x}_i]$.

- Several methods for calculating the α-values are available.

Example: a univariate nonconvex function

- The αBB underestimator for the function

$$h(x) = x \cdot \sin x + x/10$$

on the interval $0 \leq x \leq 8$ becomes

$$L(x) = h(x) + \underbrace{4.10293}_{\alpha} \cdot (0 - x)(8 - x).$$

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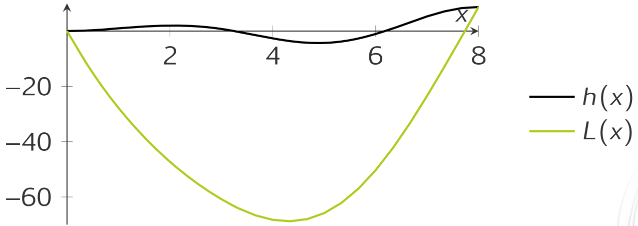
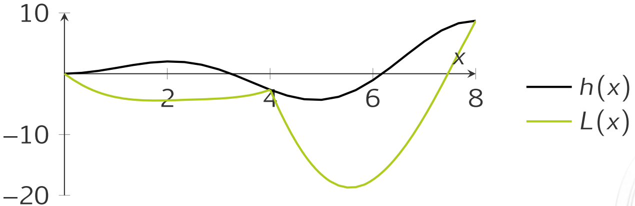


Example: The αBB underestimator

- If the domain is partitioned, new αBB underestimators (with different α-values) can be obtained in each partition, *e.g.,*

$$L(x) = \begin{cases} h(x) + 1.6 \cdot (0-x)(4-x) & \text{if } 0 \leq x \leq 4 \\ h(x) + 4.10293 \cdot (4-x)(8-x) & \text{if } 4 \leq x \leq 8 \end{cases}$$



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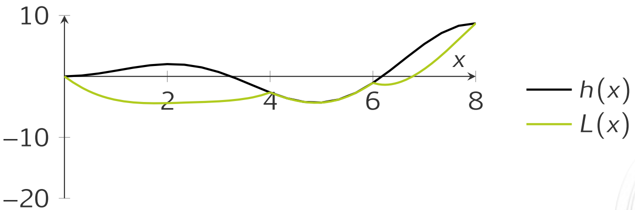

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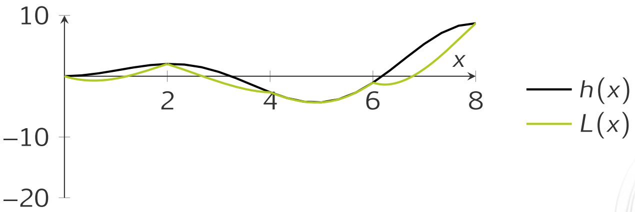
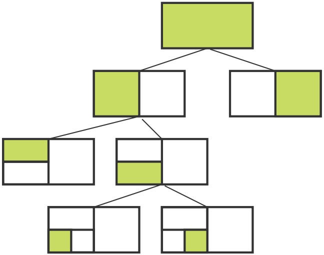
$$L(x) = \begin{cases} h(x) + 1.32544 \cdot (0-x)(4-x) & \text{if } 0 \le x \le 2 \\ h(x) + 1.6 \cdot (0-x)(4-x) & \text{if } 2 \le x \le 4 \\ h(x) & \text{if } 4 \le x \le 6 \\ h(x) + 4.10293 \cdot (6-x)(8-x) & \text{if } 6 \le x \le 8 \end{cases}$$



Branching vs reformulation



- **Branching:** *n* convex subproblems (the subproblem with the green domains are solved in each node)
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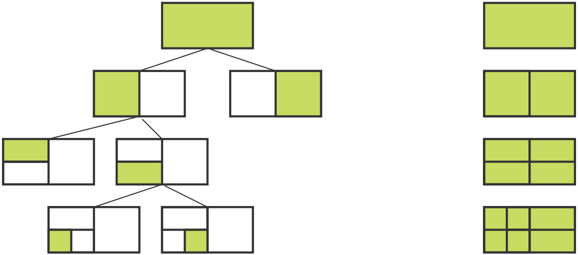

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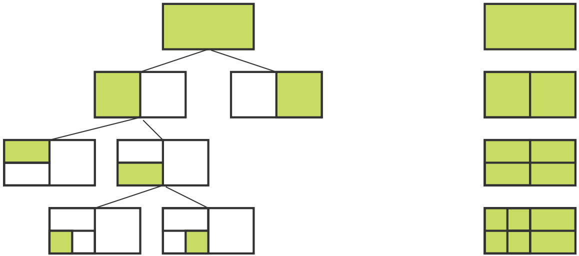

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Including the αBB underestimator into the framework

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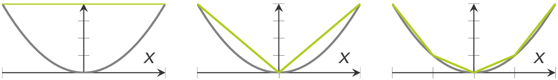
- The function αx^2 must be convex enough to overpower any nonconvexities in the variable range.

Convex reformulation of the constraints

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



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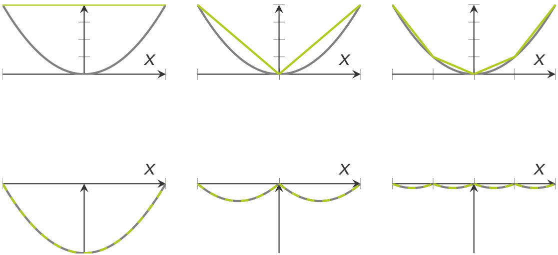

- If α in αx^2 is large enough then $h(x) + \alpha x^2 - \widehat{W}$ will be convex.
- If $\widehat{W}$ is a PLF of αx^2 then $h(x)$ is underestimated since $\alpha x^2 - \widehat{W} \leq 0$.

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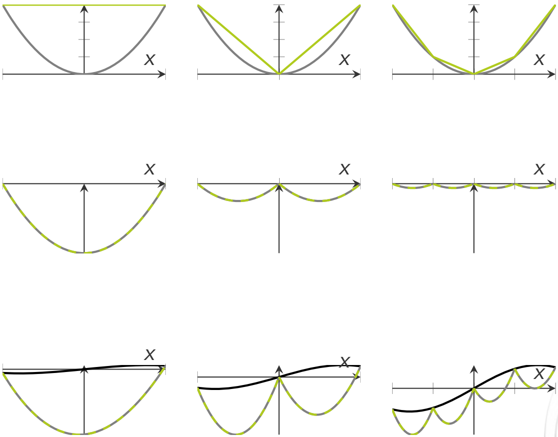

Pros and cons for the reformulation technique

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$$\alpha = \max_k \alpha_k,$$

where α_k is the minimal α-value needed for convexification in the k-th breakpoint interval of the PLFs.

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– If the αBB underestimator is used in this form in the reformulation framework, α cannot be zero in intervals where the function is convex.

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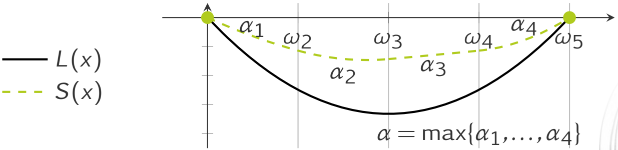
  - different α-values in different subintervals can be used
  - α can be zero in intervals where the function is convex
- The spline αBB underestimator is a smooth (continuously differentiable) piecewise quadratic convex function.
- Originally the spline underestimator was developed for improving the αBB underestimators in subsubdomains (Meyer and Floudas, 2005).
  - This property of the spline can be utilized in the reformulation framework as well.

The spline αBB underestimator

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

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

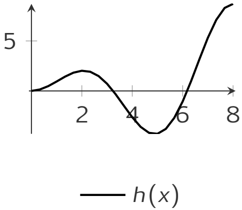
- The α_k's ensure convexity. The β_k and γ_k for $k \in \{2, \ldots, K-1\}$ ensure smoothness and continuity, and β_1, γ_1 gives $S(\omega_1) = S(\omega_K) = 0$.



An illustrative example

- Consider now the same function as before

$$h(x) = x \cdot \sin x + x/10.$$



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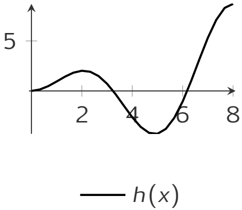

- The convex underestimators are then

$$\hat{h}_1(x) = x \cdot \sin x + x/10 + \alpha x^2 - \widehat{W}$$

for the reformulated original αBB understimator and

$$\hat{h}_2(x) = x \cdot \sin x + x/10 + S(x) - \widehat{S}$$

for the reformulated spline αBB underestimator, where $\widehat{W}$ is the PLF of $W = \alpha x^2$ and $\widehat{S}$ is the PLF of the spline function $S(x)$.

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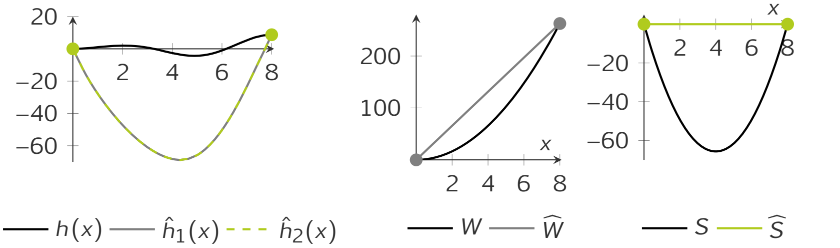

$$\hat{h}_1(x) = x \cdot \sin x + x/10 + \boxed{\alpha x^2 - \widehat{W}} \qquad \alpha = 4.10293$$

$$\hat{h}_2(x) = x \cdot \sin x + x/10 + \boxed{S(x) - \widehat{S}}$$

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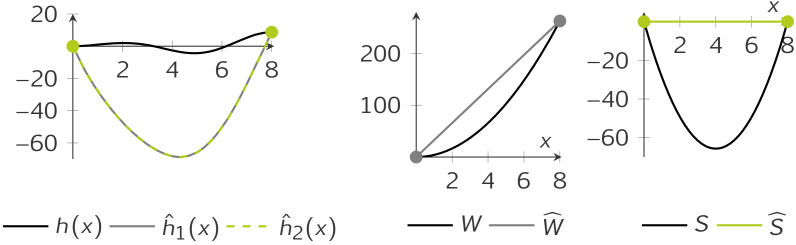

$$W(x) = 4.1x^2 \qquad S(x) = 4.1x^2 - 32.8x, 0 \leq x \leq 8$$

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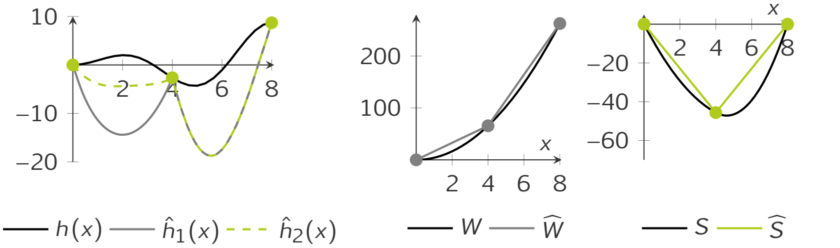
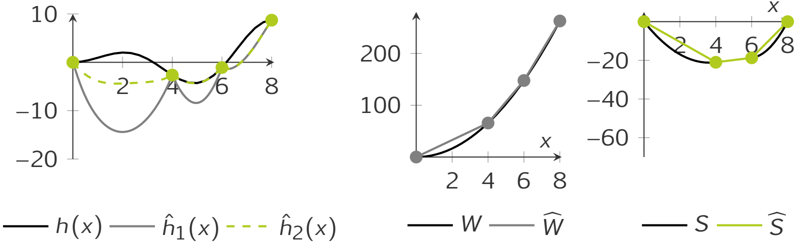


$$W(x) = 4.1x^2 \qquad S(x) = \begin{cases} 1.6x^2 - 17.8x & 0 \leq x \leq 4 \\ 4.1x^2 - 37.8x + 40.0 & 4 \leq x \leq 8 \end{cases}$$

An illustrative example



$$W(x) = 4.1x^2 \qquad S(x) = \begin{cases} 1.6x^2 - 11.7x & 0 \le x \le 4 \\ 1.1x - 25.6 & 4 \le x \le 6 \\ 4.1x^2 - 48.1x + 122.1 & 6 \le x \le 8 \end{cases}$$

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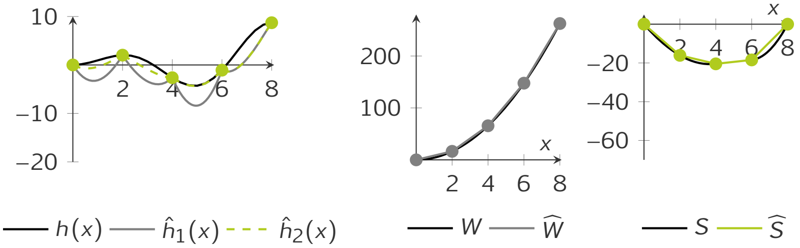

$$W(x) = 4.1x^2 \qquad S(x) = \begin{cases} 1.3x^2 - 10.7x & 0 \leq x \leq 2 \\ 1.6x^2 - 11.8x + 1.1 & 2 \leq x \leq 4 \\ 1.1x - 24.5 & 4 \leq x \leq 6 \\ 4.1x^2 - 48.2x + 123.2 & 6 \leq x \leq 8 \end{cases}$$

Generalization to N dimensions

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

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

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

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

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- 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.

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- A sequence of overestimated convex MINLP problems is solved until the solution fulfills the constraints in the original nonconvex problem.
- The overestimated feasible region of the convexified problems (in the original variables) is reduced in each iteration by improving the PLFs of $W = \alpha_i x_i^2$ or $S(x)$.

The original nonconvex MINLP problem

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

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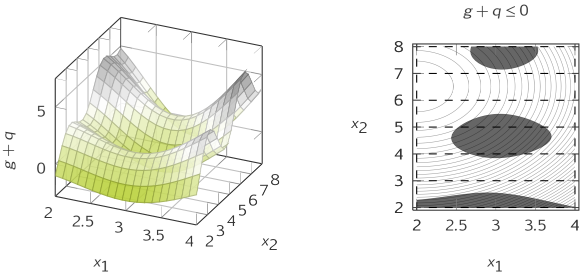


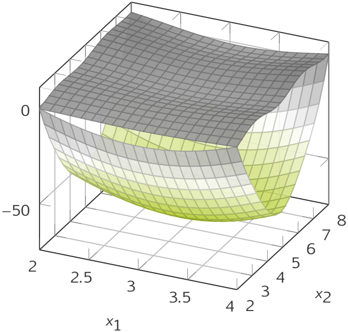
The reformulated MINLP problem

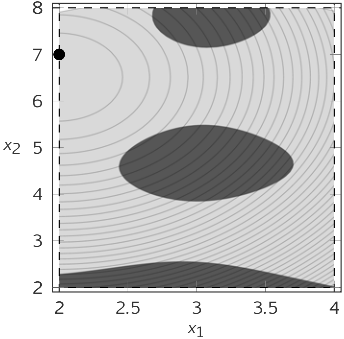
$$\begin{aligned} &\text{minimize} && f(x_1,x_2) = (2x_1-4)^2 + (x_2-13/2)^2 \\ &\text{subject to} && x_1\cos^2 x_2 + x_2 \sin^2 x_1 - 3/x_2 + x_1/2 - 5/2 \\ & && \qquad + S_1(x_1) + S_2(x_2) - \widehat{S}_1 - \widehat{S}_2 \leq 0, \\ & && \widehat{S}_1 = \mathrm{PLF}(S_1(x_2), V_1;\, \Omega_1),\ \widehat{S}_2 = \mathrm{PLF}(S_2(x_2), V_2;\, \Omega_2), \\ & && 2 \leq x_1 \leq 4, \quad 2 \leq x_2 \leq 8, \quad x_1 \in \mathbb{R}, \quad x_2 \in \mathbb{Z}, \end{aligned}$$

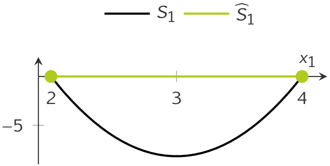
V_i and Ω_i are sets including the variables and breakpoints in PLF_i of $S_i(x_1)$

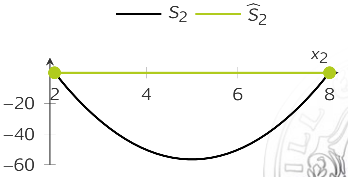
- This reformulated problem is convex in the extended variable space consisting of the original variables x_1 and x_2, as well as, those needed for the PLFs in V_1 and V_2.

αGO iteration 1

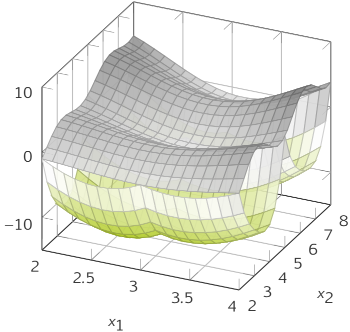


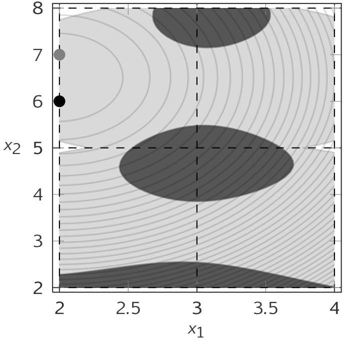


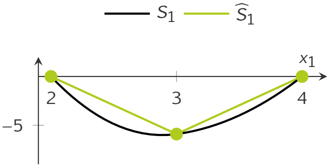


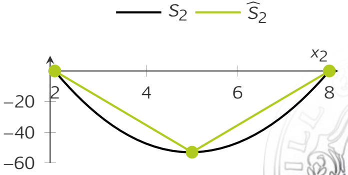


αGO iteration 2









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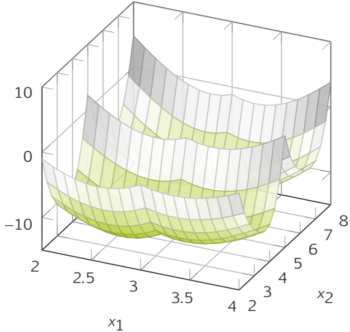
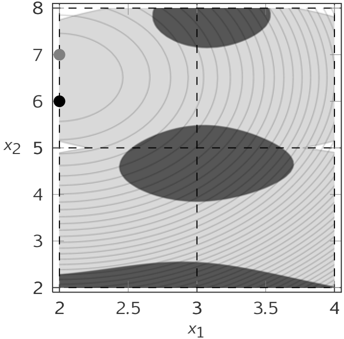
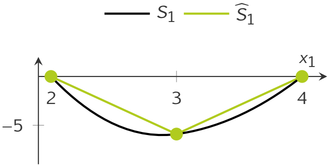
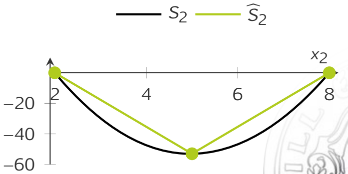
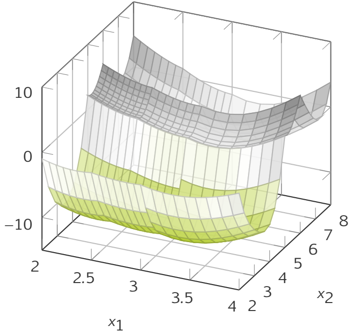


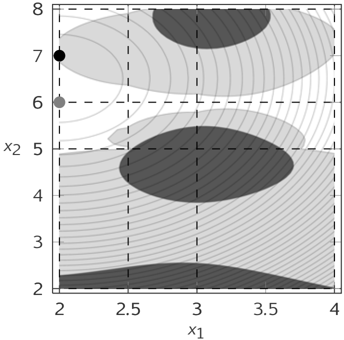


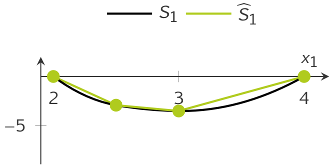


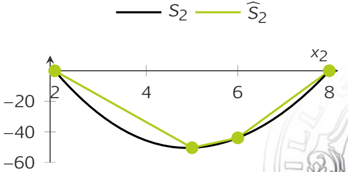


αGO iteration 3

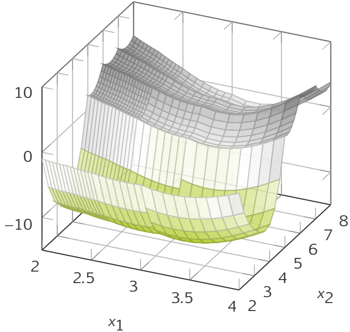


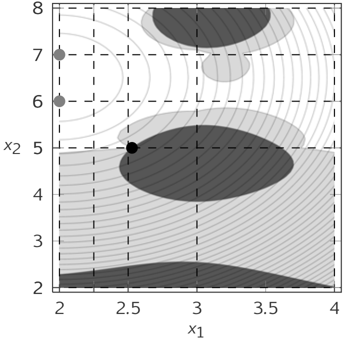


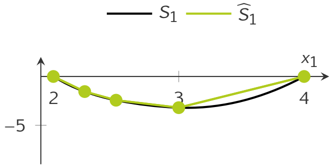


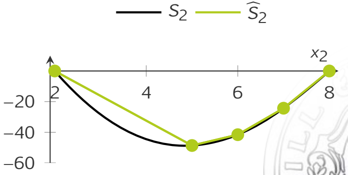


αGO iteration 4

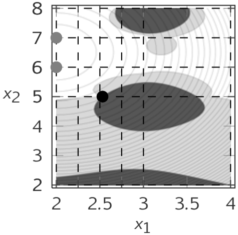


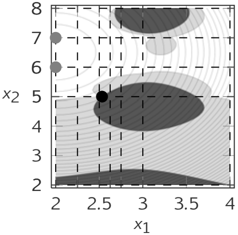






αGO iteration 5 and 6





Iter.	Regions	$f(x_1, x_2)$	x_1	x_2	$g(x_1, x_2) + q(x_1)$
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

On-going and future work

- Exclusion of infeasible regions by, *e.g.,* interval arithmetic and integer cuts

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- Numerical studies

Summary

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- αGO/SGO is a global optimization algorithm for nonconvex twice-differentiable MINLP problems.
  - The αBB underestimator is used to handle the nonconvex C^2-functions.
- In the algorithm no direct branching strategy is needed for handling the nonconvexities, instead a reformulated and convexified MINLP problem is solved iteratively until the global solution is found.
- Easy to implement, since only a method for calculating the α-values and a convex MINLP solver is needed.

Some references

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The end of the presentation

Thank you for listening!

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Questions?