Global Optimization methods for Mixed Integer Non Linear Programs with Separable Non Convexities

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Outline

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Introduction on MINLP

Mixed Integer Non Linear Programming problem:

$$\begin{aligned} &\min c(x) & \\ &\quad f_i(x) \leq 0 & \forall i \in M \\ &\quad L_j \leq x_j \leq U_j & \forall j \in N \\ &\quad x_j \text{ integer} & \forall j \in I \end{aligned}$$

where c and f are **twice continuously differentiable functions** .

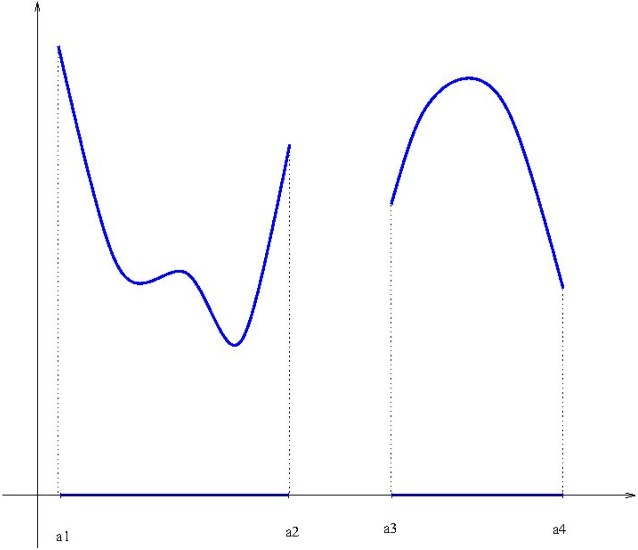
Bounds on variables are important.

Spatial Branch-and-Bound

30 years ago: first general-purpose "exact" algorithms for nonconvex MINLP.

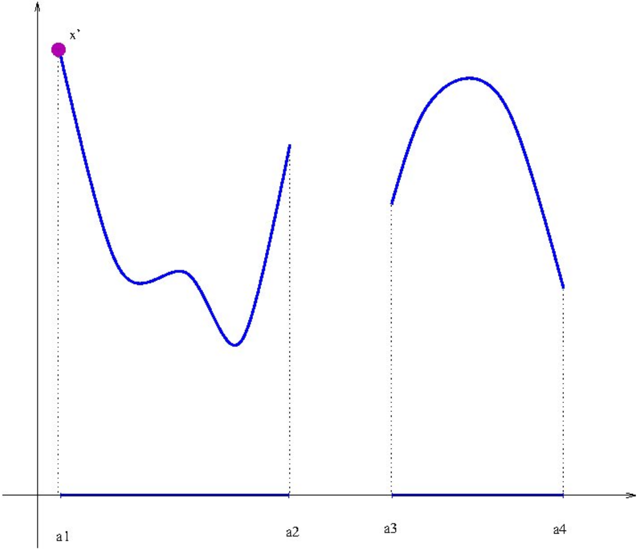
- Tree-like search
- Explores search space exhaustively but implicitly
- Builds a sequence of decreasing upper bounds and increasing lower bounds to the global optimum
- Exponential worst-case
- Only general-purpose "exact" algorithm for MINLP
  Since continuous vars are involved, should say "ε-approximate"
- Like BB for MILP, but may branch on continuous vars
  Done whenever one is involved in a nonconvex term

Spatial B&B: Example



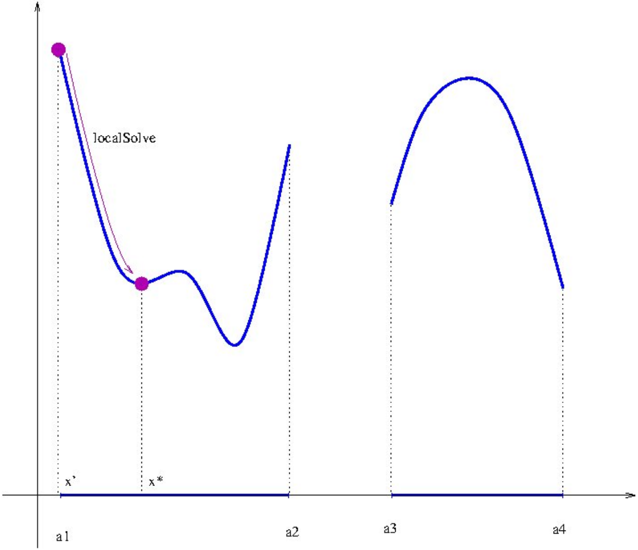
Original problem P

Spatial B&B: Example



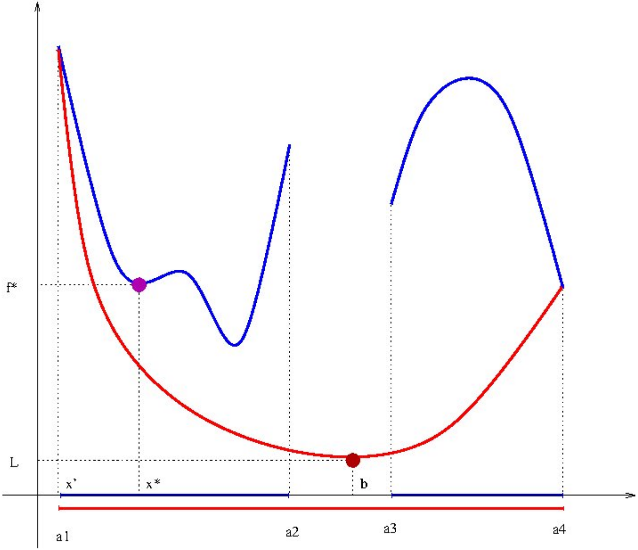
Starting point x'

Spatial B&B: Example



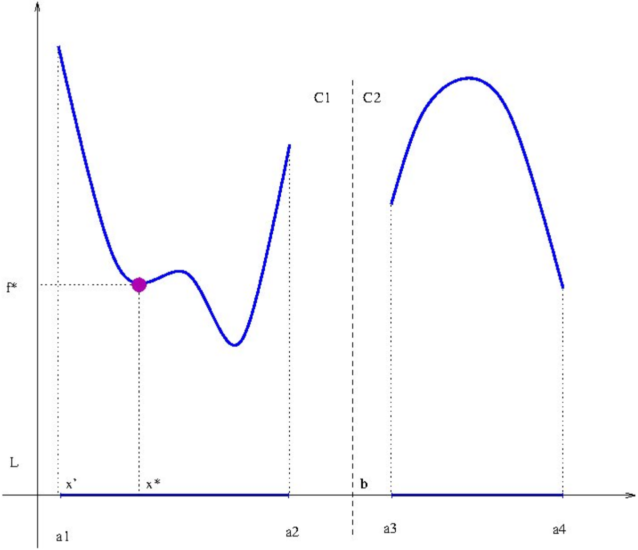
Local (upper bounding) solution x^*

Spatial B&B: Example



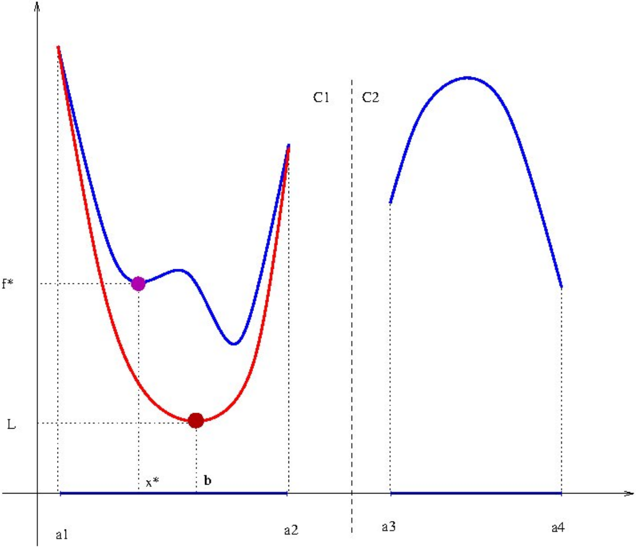
Convex relaxation (lower) bound $\bar{f}$ *with* $|f^* - \bar{f}| > \varepsilon$

Spatial B&B: Example



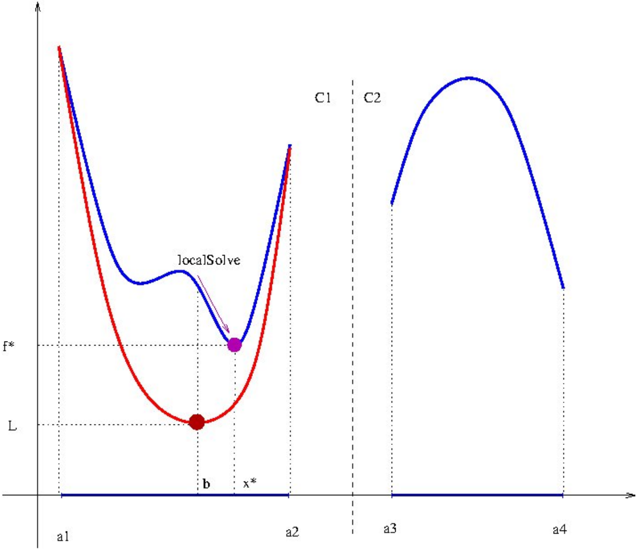
Branch at $x = \bar{x}$ *into* C_1, C_2

Spatial B&B: Example



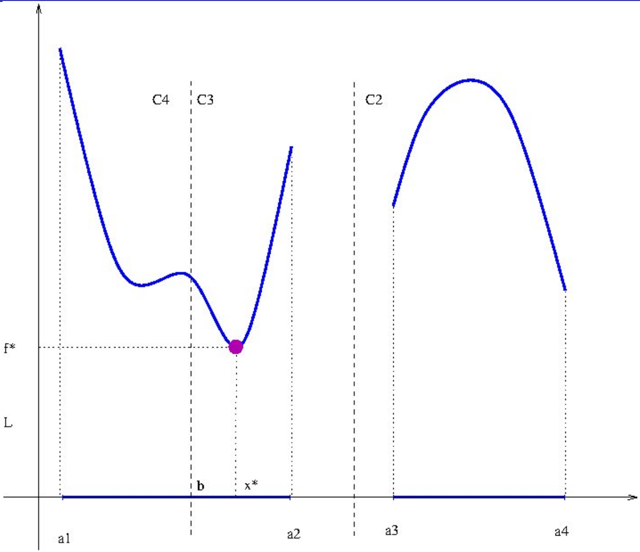
Convex relaxation on C_1: lower bounding solution $\bar{x}$

Spatial B&B: Example



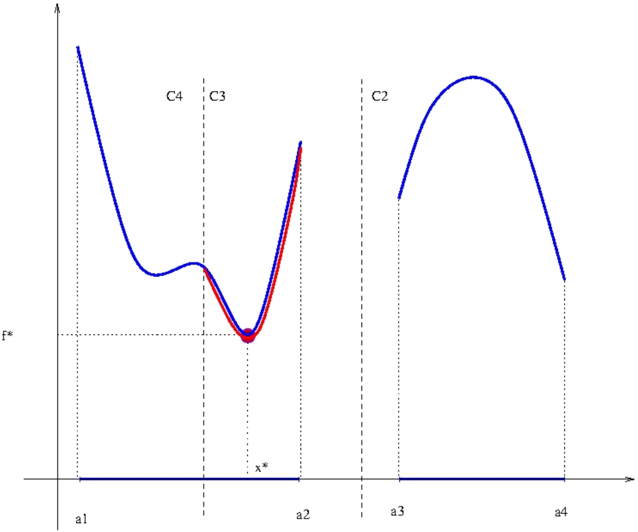
localSolve. *from $\bar{x}$: new upper bounding solution x^**

Spatial B&B: Example



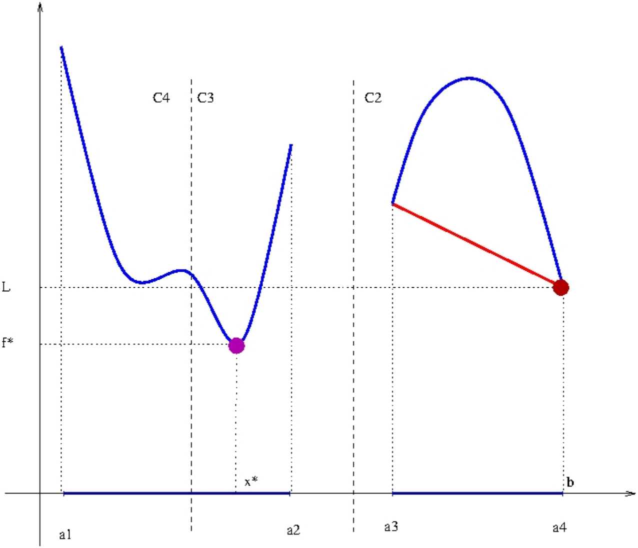
$$|f^* - \bar{f}| > \varepsilon\text{: branch at } x = \bar{x}$$

Spatial B&B: Example



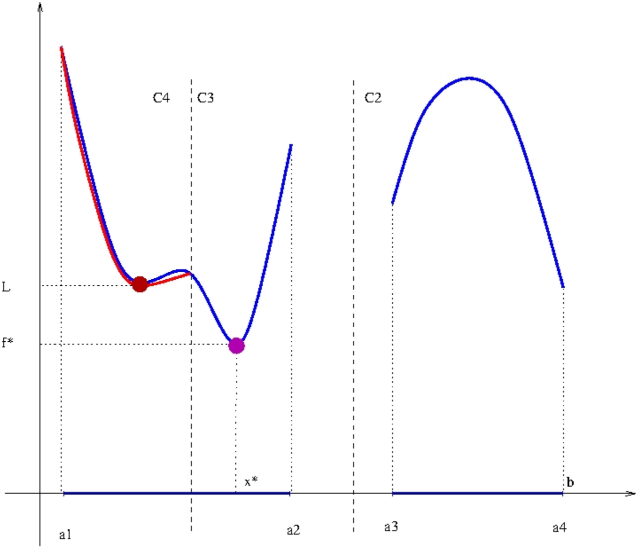
Repeat on C_3: get $\bar{x} = x^*$ and $|f^* - \bar{f}| < \varepsilon$, no more branching

Spatial B&B: Example



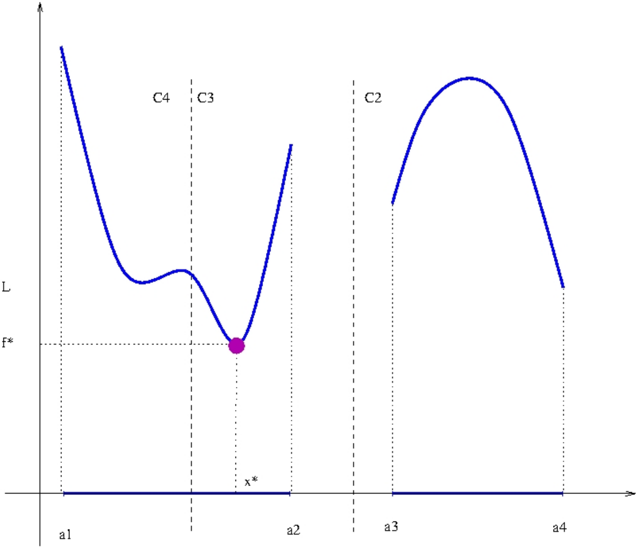
Repeat on C_2: $\bar{f} > f^*$ (can't improve x^* in C_2)

Spatial B&B: Example



Repeat on C_4: $\bar{f} > f^*$ (can't improve x^* in C_4)

Spatial B&B: Example



No more subproblems left, return x^* and terminate

Spatial B&B: Pruning

- Search generates a tree
- Suproblems are nodes
- Nodes can be pruned by optimality, bound or **infeasibility** (when subproblem is infeasible)
- Otherwise, they are branched
- Whole space explored

Spatial B&B: General idea

Aimed at solving “factorable functions”, i.e., f and c of the form:

$$\sum_h \prod_k f_{hk}(x, y)$$

where $f_{hk}(x, y)$ are $\in$ {sum, product, quotient, power, exp, log, sin, cos, abs} $\forall h, k$.

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- **Relax (linear/convex)** the basic nonlinear terms (library of envelopes/underestimators).

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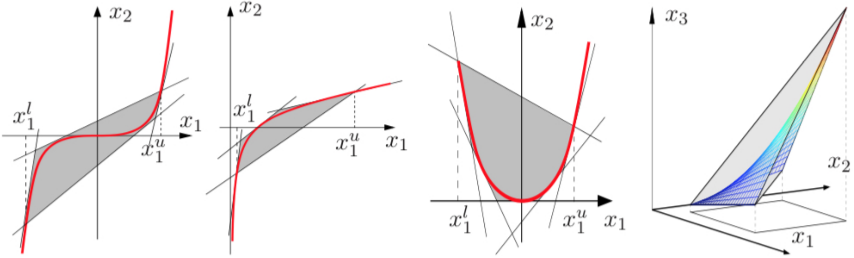
- **Exact reformulation** of MINLP so as to have "isolated basic nonlinear functions" (additional variables and constraints).
- **Relax (linear/convex)** the basic nonlinear terms (library of envelopes/underestimators).
- Relaxation depends on variable bounds, thus **branching** potentially strengthen it.



(a) $x_2 = x_1^3$ (b) $x_2 = \log x_1$ (c) $x_2 = x_1^2$ (d) $x_3 = x_1 x_2$

P. Belotti, J. Lee, L. Liberti, F. Margot, A. Wächter, “Branching and bounds tightening techniques for non-convex MINLP”. Optimization Methods and Software 24(4-5): 597-634 (2009).

Outline

The class of MINLP problems

$$\min \sum_{j \in N} C_j x_j$$

$$f_i(x) + \sum_{k \in H_i} g_{ik}(x_k) \leq 0 \qquad \forall i \in M$$

$$L_j \leq x_j \leq U_j \qquad \forall j \in N$$

$$x_j \text{ integer} \qquad \forall j \in I$$

where:

- $f_i : \mathbb{R}^n \to \mathbb{R}$ are convex functions $\forall i \in M$,
- $g_{ik} : \mathbb{R} \to \mathbb{R}$ are non convex univariate function $\forall i \in M, \forall k \in H_i$,
- $H_i \subseteq N \;\; \forall i \in M$,
- $I \subseteq N$, and
- L_j and U_j are finite $\forall i \in M, j \in H_i$

Outline

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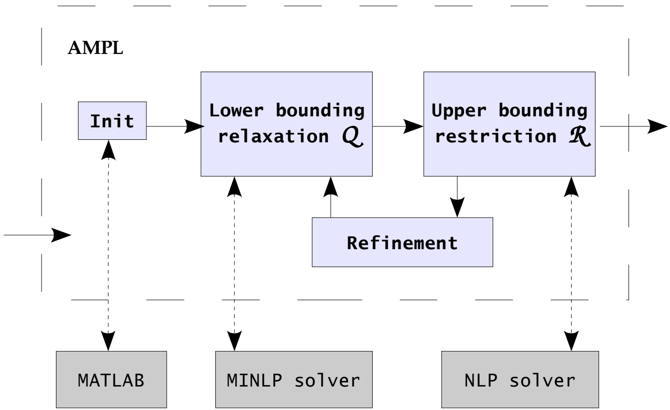
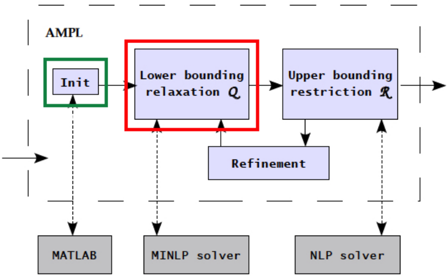
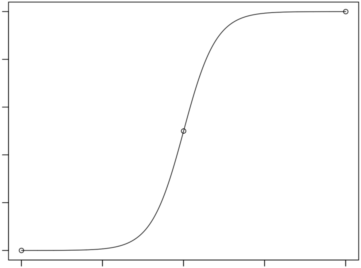
General Framework

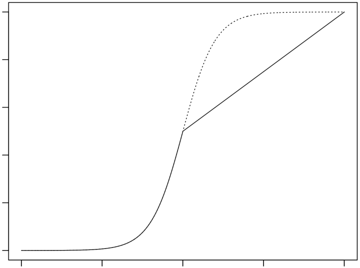
Global optimization algorithm proposed in D'A., Lee, and Wächter (2009, 2012).



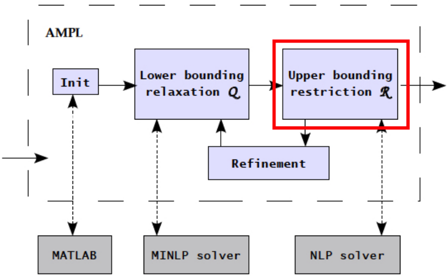
General Framework





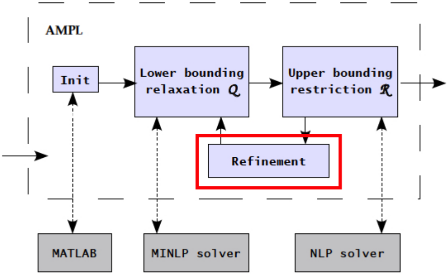


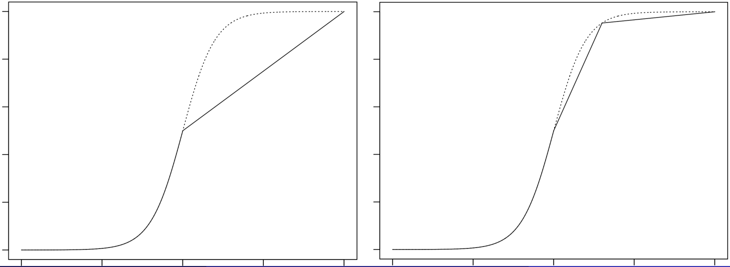
General Framework



Fix the value of the integer variables $\rightarrow$ nonconvex NLP

General Framework





Outline

The Upper Bounding problem

Upper Bound of the original problem:

1. The integer variables are fixed;
2. We solve the resulting non convex NLP problem to local optimality;

$$\min \sum_{j \in N} C_j x_j$$

$$f_i(x) + \sum_{k \in H_i} g_{ik}(x_k) \leq 0 \qquad \forall i \in M$$

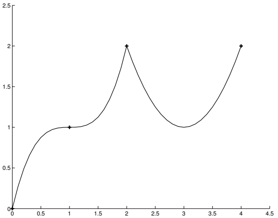
$$L_j \leq x_j \leq U_j \qquad \forall j \in N$$

$$x_j = \underline{x}_j \qquad \forall j \in I$$

Outline

The Lower Bounding problem: step 1

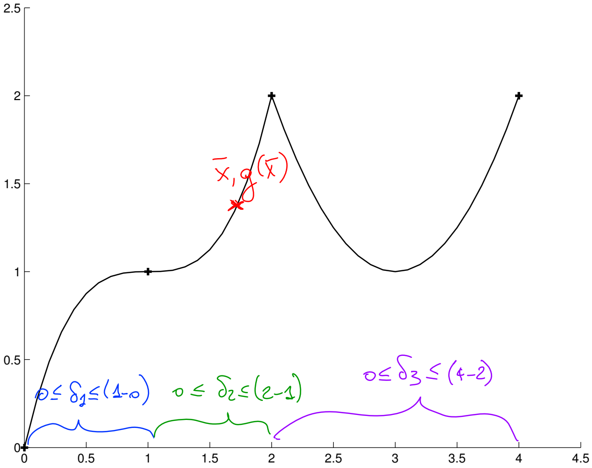
For simplicity, let us consider a term of the form $g(x_k) := g_{ik}(x_k)$: $g : \mathbb{R} \to \mathbb{R}$ is a univariate non convex function of x_k , for some k ($1 \leq k \leq n$).



Automatically detect the concavity/convexity intervals or piecewise definition:
$[P_{p-1}, P_p]$:= the p-th subinterval of the domain of g ($p \in \{1 \ldots \overline{p}\}$);
$\check{H}$:= the set of indices of subintervals on which g is convex;
$\hat{H}$:= the set of indices of subintervals on which g is concave.

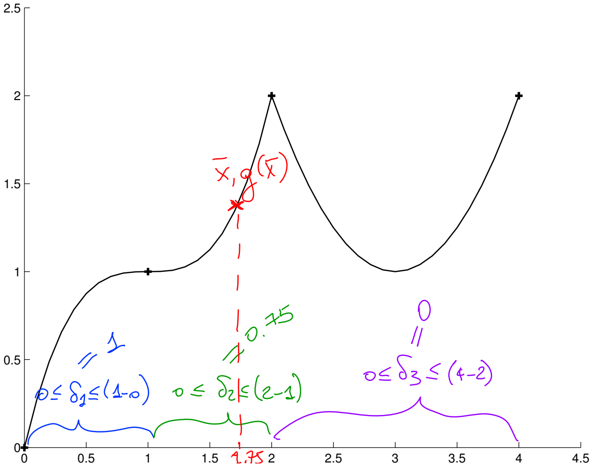
The Lower Bounding problem: step 2

Introduction of additional variables $\delta_p \in [0, P_p - P_{p-1}]$ such that $x_k = P_0 + \sum_{p=1}^{\bar{p}} \delta_p$



The Lower Bounding problem: step 2

Introduction of additional variables $\delta_p \in [0, P_p - P_{p-1}]$ such that $x_k = P_0 + \sum_{p=1}^{\bar{p}} \delta_p = 0 + 1 + 0.75 + 0$



The Lower Bounding problem: step 2

- All the δ's but at most 1 take either the lower or the upper bound value
- To model such behavior additional binary variables are needed: $z_p \in \{0,1\}\ \forall p$
- $z_1 \geq z_2 \geq \cdots \geq z_p$
- $\delta_p = \begin{cases} 0 & z_{p-1} = 0 \\ [0, P_p - P_{p-1}] & z_{p-1} = 1 \text{ and } z_p = 0 \\ P_p - P_{p-1} & z_p = 1 \end{cases}$

δ	$P_1 - P_0$	$P_2 - P_1$	$\dots$	$P_{p-1} - P_{p-2}$	$[0, P_p - P_{p-1}]$	0	$\dots$	0
z	1	1	$\dots$	1	0	0	$\dots$	0

The Lower Bounding problem: step 2

Replace the term $g(x_k)$ with:

$$\sum_{p=1}^{\bar{p}} g(P_{p-1} + \delta_p) - \sum_{p=1}^{\bar{p}-1} g(P_p) \ ,$$

and we include the following set of new constraints:

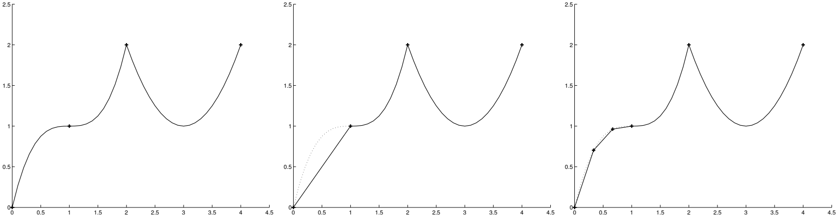
$$x_k = P_0 + \sum_{p=1}^{\bar{p}} \delta_p \ ;$$
$$\delta_p \geq (P_p - P_{p-1}) z_p \ , \ \forall p \in \check{H} \cup \hat{H} \ ;$$
$$\delta_p \leq (P_p - P_{p-1}) z_{p-1} \ , \ \forall p \in \check{H} \cup \hat{H} \ ;$$
$$0 \leq \delta_p \leq P_p - P_{p-1}, \ \forall p \in \{1, \ldots, \bar{p}\};$$

with two dummy variables $z_0 := 1$ and $z_{\bar{p}} := 0$ and two new sets of variables z_p (binary) and δ_p (continuous).

The Lower Bounding problem: step 3

Still non convex;

Use piece-wise linear approximation for the concave intervals:



The Lower Bounding problem: the convex MINLP model

Replace the term $g(x_k)$ with:

$$\sum_{p\in\check{H}} g(P_{p-1}+\delta_p)+\sum_{p\in\hat{H}}\sum_{b\in B_p} g(X_{p,b})\,\alpha_{p,b}-\sum_{p=1}^{\overline{p}-1} g(P_p)\ ,$$

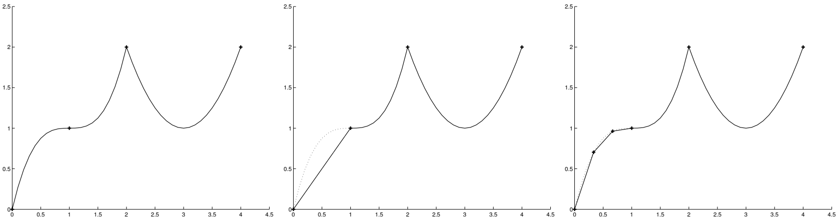
and we include the following set of new constraints:

$$\begin{aligned}
&P_0+\sum_{p=1}^{\overline{p}}\delta_p - x_k = 0\ ;\\
&\delta_p-(P_p-P_{p-1})z_p \geq 0\ ,\ \forall p\in\check{H}\cup\hat{H}\ ;\\
&\delta_p-(P_p-P_{p-1})z_{p-1} \leq 0\ ,\ \forall p\in\check{H}\cup\hat{H}\ ;\\
&P_{p-1}+\delta_p-\sum_{b\in B_p} X_{p,b}\,\alpha_{p,b}=0\ ,\ \forall p\in\hat{H}\ ;\\
&\sum_{b\in B_p}\alpha_{p,b}=1\ ,\ \forall p\in\hat{H}\ ;\\
&\{\alpha_{p,b}: b\in B_p\} := \mathrm{SOS2}\ ,\qquad \forall p\in\hat{H}\ .
\end{aligned}$$

with two dummy variables $z_0 := 1$, $z_{\overline{p}} := 0$ and the new set of variables $\alpha_{p,b}$.

Outline

Refining the Lower Bounding problem



- Add a breakpoint where the solution of problem $\mathcal{Q}$ of the previous iteration lies (global convergence);
- Add a breakpoint where the solution of problem $\mathcal{R}$ of the previous iteration lies (speed up the convergence).

Outline

Convergence Theorem

Theorem

Under mild assumptions (e.g., the non convex functions are uniformly Lipschitz-continuous), the algorithm either terminates at a global solution of the original problem, or each limit point of the sequence $\{\underline{x}^l\}_{l=1}^{\infty}$ *is a global solution of the original problem.*
($\underline{x}^l$ *= LB problem solution at iteration* l*)*

Sketch of proof:

- Ends in a finite n. iterations: either $\underline{x}^l$ is feasible for the original problem, or x_{UB} such that $UB = LB$.
- Otherwise, the basic idea: at each iteration, the error of problem $\mathcal{Q}$ is shrinked because of the first refinement rule.

Outline

Computational Results

Results for Nonlinear Continuous Knapsack problem

instance	var/int/cons original	SC-MINLP time (LB)	SC-MINLP UB	COUENNE time (LB)	COUENNE UB	BONMIN 1 time	BONMIN 1 UB	BONMIN 50 time	BONMIN 50 UB
nck_20_100	40/0/21	15.76	-159.444	3.29	-159.444	0.02	-159.444	1.10	-159.444
nck_20_200	40/0/21	23.76	-239.125	(-352.86)	-238.053	0.03	-238.053	0.97	-239.125
nck_20_450	40/0/21	15.52	-391.337	(-474.606)	-383.149	0.07	-348.460	0.84	-385.546
nck_50_400	100/0/51	134.25	-516.947	(-1020.73)	-497.665	0.08	-438.664	2.49	-512.442
nck_100_35	200/0/101	110.25	-81.638	90.32	-81.638	0.04	-79.060	16.37	-79.060
nck_100_80	200/0/101	109.22	-172.632	(-450.779)	-172.632	0.04	-159.462	15.97	-171.024

Results for Uncapacitated Facility Location problem

instance	var/int/cons original	SC-MINLP time (LB)	SC-MINLP UB	COUENNE time (LB)	COUENNE UB	BONMIN 1 time	BONMIN 1 UB	BONMIN 50 time	BONMIN 50 UB
ufl_1	45/3/48	116.47	4,330.400	529.49	4,330.400	0.32	4,330.400	369.85	4,330.400
ufl_2	45/3/48	17.83	27,516.569	232.85	27,516.569	0.97	27,516.569	144.06	27,516.569
ufl_3	32/2/36	8.44	2,292.777	0.73	2,292.775	3.08	2,292.777	3.13	2,292.775

Results for Hydro Unit Commitment and Scheduling problem

instance	var/int/cons original	SC-MINLP time (LB)	SC-MINLP UB	COUENNE time (LB)	COUENNE UB	BONMIN 1 time	BONMIN 1 UB	BONMIN 50 time	BONMIN 50 UB
hydro_1	124/62/165	107.77	-10,140.763	(-11,229.80)	-10,140.763	5.03	-10,140.763	5.75	-7,620.435
hydro_2	124/62/165	211.79	-3,932.182	(-12,104.40)	-2,910.910	4.63	-3,928.139	7.02	-3,201.780
hydro_3	124/62/165	337.77	-4,710.734	(-12,104.40)	-3,703.070	5.12	-4,131.095	13.76	-3,951.199

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Limitations

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- **Large number of iterations** needed to converge

Lower Bounding problem tightening

Let us consider the convex pieces:

$$g(P_{p-1} + \delta_p) - g(P_{p-1})$$

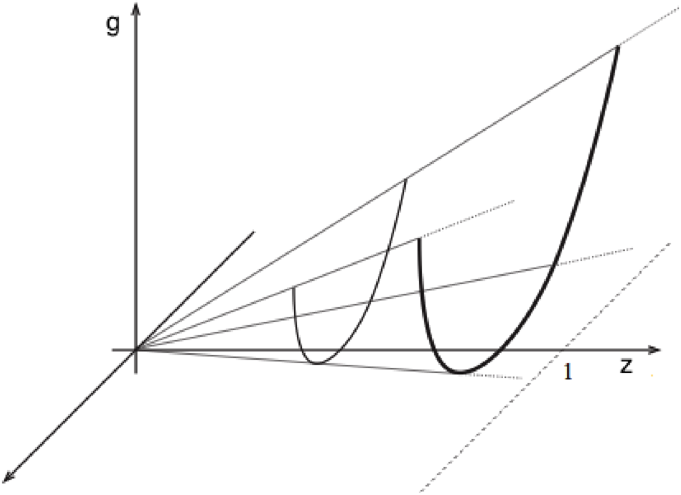
with

- $0 \leq \delta_p \leq (P_p - P_{p-1}) z_{p-1}$
- $z_{p-1} \in \{0, 1\}$

Its **convex envelope** is:

$$z_{p-1}(g(P_{p-1} + \delta_p / z_{p-1}) - g(P_{p-1}))$$

Perspective function



Where can we exploit it?

Use it to solve the Lower Bounding problem:

- Reformulate the convex MINLP
- Stronger the convex continuous relaxation
- Generate stronger linear cuts
- Solve the convex MINLP with cutting plane

More Computational Results

- PC: linearization of PR of LB problem
- STD: linearization of original LB problem
- Bonmin
- Minotaur
- SCIP

Tests on non linear knapsack problem and uncapacitated facility location problem.

10,000 seconds time limit.

Results on the non linear knapsack problem

size	PC		STD		Bonmin	MINOTAUR			SCIP
	time	cuts	time	cuts	time	time	gap	bgap	time
10	0.014	96	0.015	102	0.267	0.09	-	-	0.07
20	0.021	155	0.019	195	0.324	0.16	-	-	0.10
50	0.048	431	0.085	678	0.617	0.63	-	-	0.21
100	0.072	947	0.183	1182	1.067	3.44	-	-	0.66
200	0.105	1780	0.565	2461	2.237	28.6	-	-	131.2
500	0.380	4681	3.593	7821	8.406	7080	0.15	0.05	181.4

Table: NCK: comparison among the different algorithms

Results on the uncapacitated facility location problem

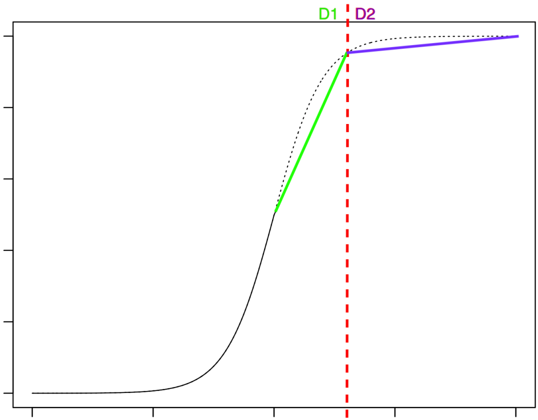
instance	PC				STD				Bonmin			Minotaur		
	time	gap	bgap	cuts	time	gap	bgap	cuts	time	gap	bgap	time	gap	bgap
6x12x1	0.35	-	-	1673	0.26	-	-	1531	1.37	-	-	4.66	-	-
6x12x2	0.45	-	-	1842	0.42	-	-	1796	5.64	-	-	65.6	-	-
6x12x3	7921	-	-	33417	tl	54.3	52.4	180561	tl	657	796	tl	260	615
12x24x1	3.36	-	-	9565	2.55	-	-	8971	7.14	-	-	57.4	-	-
12x24x2	46.1	-	-	19653	27.3	-	-	17384	57.9	-	-	tl	17.4	10.5
12x24x3	tl	23.9	23.9	127380	tl	121	134	284557	tl	∞	1524	tl	272	1447
24x48x1	261	-	-	81372	316	-	-	102160	116	-	-	2844	-	-
24x48x2	tl	5.93	5.67	164809	tl	9.66	9.66	409177	tl	73.4	26.4	tl	31.5	24.6

Table: UFL: Comparison among different algorithms

Limitations

- Solving the Lower Bounding problem can be **time consuming**
- At each iteration we solve the Lower Bounding problem **from scratch**
- **Large number of iterations** needed to converge

Disjunctive Cuts



$\psi \in (0, P_k - P_{k-1})$

- $\mathbf{D_1} \rightarrow \delta_k \leq \psi$ and ———
- $\mathbf{D_2} \rightarrow \delta_k \geq \psi$ and ———

Disjunctive Cuts

Strengthening

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IDC $\{\mathbf{D_1} \wedge z_k = 0\} \vee \{\mathbf{D_2} \wedge z_{k-1} = 1\}$

Computational Results

$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j$

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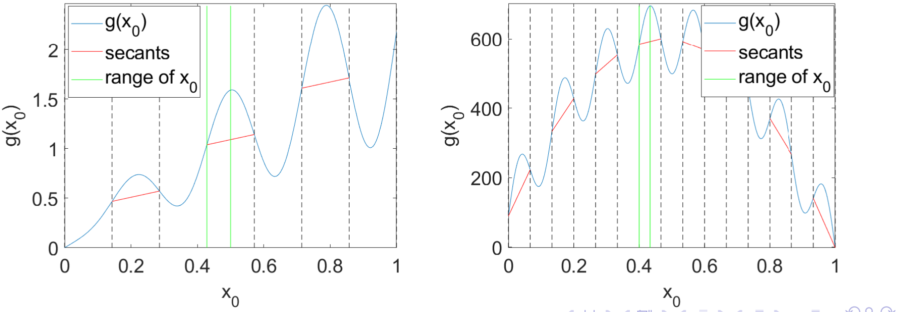
$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j$
$g(x_0) =$

1. $s \cdot x_0 - \frac{2\cos(h\pi x_0)}{h\pi} - x_0 \sin(h\pi x_0)$, and
2. $d(\sin((h\pi x_0) + 2e\pi + \sin^{-1}(\frac{m}{d}))) + m((h\pi x_0) + 2e\pi + \sin^{-1}((\frac{m}{d}))^2 + v((h\pi x_0) + 2e\pi + \sin^{-1}(\frac{m}{d}))$,

s randomly generated (uniform distribution) on $[-4, +4]$, h on $[7, 15]$, d on $\{100, 200, 300\}$, e on $\{-3, -2\}$, m on $\{-2, -1\}$, v on $\{10, 15, 20\}$.



Computational Results

inst.	strategy	CMINLP	#iter.
1	Alg	1.07	18
1	Alg+PC	1.07	12
1	Alg+IDC	**1.11**	69
2	Alg	2.09	36
2	Alg+PC	**2.15**	22
2	Alg+IDC	2.09	38
3	Alg	2.56	221
3	Alg+PC	2.57	60
3	Alg+IDC	**2.66**	300
4	Alg	**-2.10**	300
4	Alg+PC	**-2.10**	29
4	Alg+IDC	-2.13	26
5	Alg	2.70	73
5	Alg+PC	**2.72**	63
5	Alg+IDC	2.70	300

inst.	strategy	CMINLP	#iter.
6	Alg	502.44	300
6	Alg+PC	**506.85**	300
6	Alg+IDC	502.44	300
7	Alg	502.48	300
7	Alg+PC	**505.81**	300
7	Alg+IDC	502.92	300
8	Alg	246.46	300
8	Alg+PC	**252.14**	300
8	Alg+IDC	246.46	300
9	Alg	504.40	300
9	Alg+PC	504.40	300
9	Alg+IDC	504.40	300
10	Alg	587.70	300
10	Alg+PC	587.70	300
10	Alg+IDC	**589.60**	300

Computational Results

	Alg			Alg+PC			Alg+IDC		
inst.	GAP1	GAP2	GAP3	GAP1	GAP2	GAP3	GAP1	GAP2	GAP3
1	4.25	4.25	81.43	8.38	8.38	79.01	2.42	4.25	29.67
2	15.62	15.62	80.78	22.70	27.06	79.72	15.62	15.62	79.54
3	4.57	4.57	98.28	8.27	8.88	79.39	0.83	4.57	18.82
4	0.34	1.96	80.37	0.69	3.96	74.37	1.66	1.96	76.91
5	88.34	88.34	99.38	94.36	94.47	99.21	88.34	88.34	93.10
6	7.34	7.34	93.26	12.33	13.63	92.24	7.34	7.34	41.12
7	8.20	8.20	89.62	14.31	14.88	92.74	8.16	8.20	42.62
8	9.77	9.77	93.16	17.02	17.61	90.73	9.77	9.77	50.65
9	7.32	7.32	92.70	15.19	15.19	86.48	7.32	7.32	74.71
10	4.08	4.08	93.85	8.31	8.31	88.87	3.93	4.08	47.93

$GAP1 := 100 \cdot \frac{GO-CMINLP}{GO-NLP}$ $\quad GAP2 := 100 \cdot \frac{GO-MINLP}{GO-NLP}$ $\quad GAP3 := 100 \cdot \frac{GO-CNLP}{GO-NLP}$

GO: global optimum
(MI)NLP: convex (MI)NLP solution

C(MI)NLP: convex (MI)NLP solution after applying Disj. cuts

Outline

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Thanks!

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