LaGO

Branch and Cut for nonconvex block-separable MINLPs in the absence of algebraic formulations

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GICOLAG, ESI, 7.12.2006

Lagrangian Global Optimizer

General purpose solver for sparse, block-separable, nonconvex MINLPs (not rigorous, partially heuristic)

- **2000** Development started by Ivo Nowak as a solver for nonconvex MIQQPs based on Lagrangian decomposition and semidefinite relaxation
- **2001-2004** Project funded by German Science Foundation: extension to MINLP solver
- **2006** start of COIN-OR project, LaGO code becomes public
- **now** Linear-relaxation based Branch and Cut algorithm version 0.2 (work in progress)

Webpage: `https://projects.coin-or.org/LaGO`

Book: Ivo Nowak, Relaxation and Decomposition Methods for Mixed Integer Nonlinear Programming, Birkhäuser 2005

Paper: LaGO - a (heuristic) Branch and Cut algorithm for nonconvex MINLPs, submitted 2006

Overview

Preprocessing

Underestimators and Cuts

Boxreduction

Numerical Experiments

Further developments

MINLP

We consider problems of the form

$$\begin{array}{lll} \text{minimize} & c^T x & \\ \text{such that} & h_i(x) \leq 0, & i \in I, \\ & h_j(x) = 0, & j \in E, \\ & x_k \in \{0,1\}, & k \in B, \\ & x \in [\underline{x}, \bar{x}] & \end{array}$$

$-\infty < \underline{x}_i \leq \bar{x}^i < \infty$, $i \in \{1, \ldots, n\}$, $c \in \mathbb{R}^n$

- $h \in C^2\left([\underline{x}, \bar{x}], \mathbb{R}^{|I|+|E|}\right)$ are black-box functions
  LaGO needs
  - methods for the evaluation of values, gradients, and Hessians
  - optional: sparsity of jacobian, interval-arithmetic evaluations
- LaGO interfaces problems via GAMS and AMPL

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$$h_i(x) = \mathrm{const} + b^T x_L + \sum_k x_{Q_k}^T A_k x_{Q_k} + \sum_r g_r(x_{N_r})$$

for "small" disjunctive subsets Q_k and N_r of $\{1, \ldots, n\}$

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  - bounding box for still unbounded variables by "guessing"

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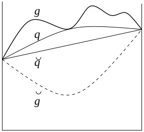
- Initialization of relaxations:



1. quadratic (nonconvex) underestimator q
2. quadratic convex underestimator $\breve{q}$
3. linearization, dropping of binary conditions

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Nonconvex quadratic underestimators

Let $g \in C^2([\underline{x}, \bar{x}], \mathbb{R})$ be nonquadratic and nonconvex.

Compute an underestimator $q(x) = x^T A x + b^T x + c$ by

$$\begin{aligned} \min_{A,b,c} \quad & \sum_{x \in S} g(x) - q(x) & \\ \text{such that} \quad & q(x) \leq g(x) & x \in S \\ & q(\hat{x}) = g(\hat{x}) & \end{aligned}$$

for a sample set $S \subseteq [\underline{x}, \bar{x}]$ and a reference point $\hat{x}$.

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- Quality of $q(x)$ depends strongly on the choice of the sample set S

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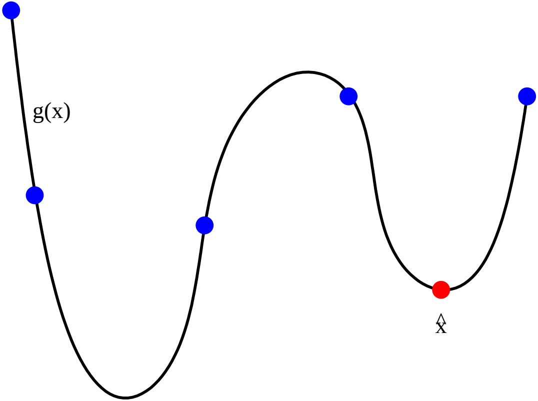
$\Rightarrow$ A. Neumaier 2006: adaptive choice of S

Nonconvex quadratic underestimator (cont.)

- initial choice: $S = \text{vert}([\underline{x}, \bar{x}]) \cup \left\{x_{\min}, \frac{1}{2}(\underline{x} + \bar{x})\right\} \cup M$ with $\hat{x} := x_{\min}$ a local minimum of $g(x)$ and M a set of random points



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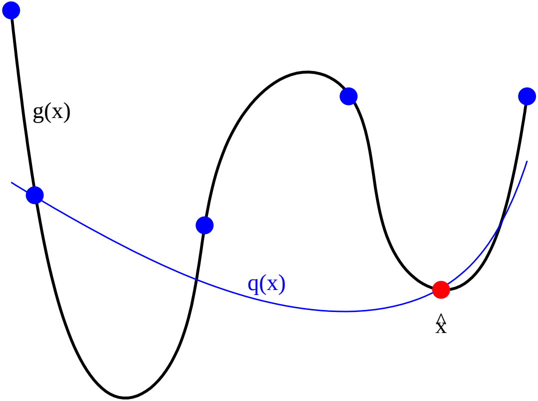
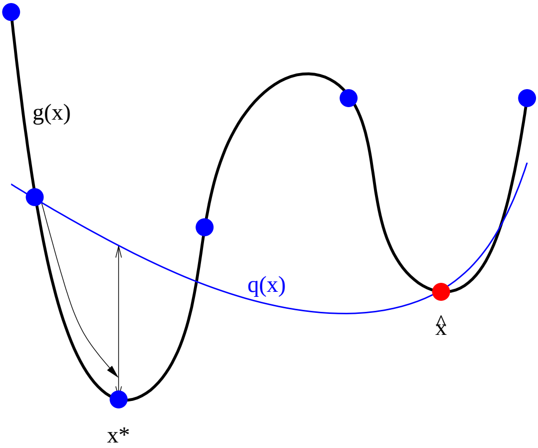


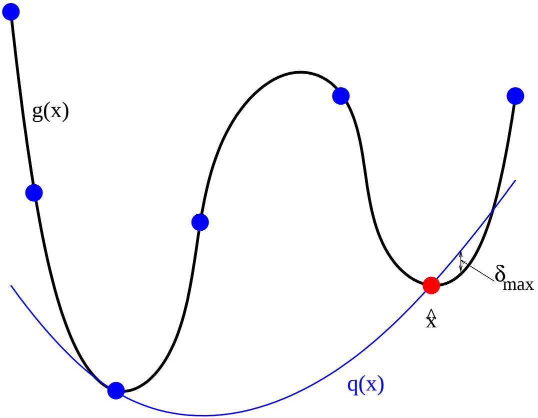
Nonconvex quadratic underestimator (cont.)

- for $x \in S$ with $g(x) = q(x)$, maximize the error $q(x) - g(x) \Rightarrow x^*$
- if $q(x^*) - g(x^*) > \delta_{\text{tol}}$, add x^* to S and recompute $q(x)$

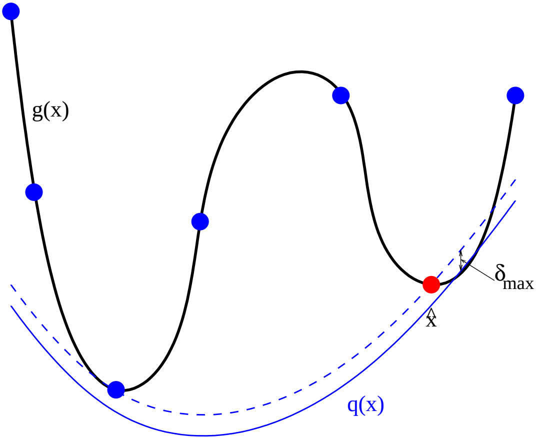


Nonconvex quadratic underestimator (cont.)

- for $x \in S$ with $g(x) = q(x)$, maximize error $q(x) - g(x) \Rightarrow \delta_{\max}$
- if $\delta_{\max} < \delta_{\text{tol}}$, lower $q(x)$ by $\delta_{\max}$



Nonconvex quadratic underestimator (cont.)



- currently only one underestimator per function and no update in Branch and Cut

Convex underestimators

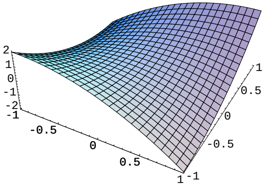
Let $q(x) = x^T A x + b^T x + c$ be a quadratic nonconvex function.

A convex α-underestimator (Adjiman and Floudas 1997) of $q(x)$ is

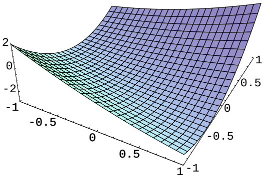
$$\breve{q}(x) = q(x) + \sum_{i=1}^{n} \alpha_i (x_i - \underline{x}_i)(x_i - \bar{x}_i)$$

where

$$\alpha_i = -\lambda_1 \left(\mathrm{Diag}(\bar{x} - \underline{x})\ A\, \mathrm{Diag}(\bar{x} - \underline{x})\right)\ (\bar{x}_i - \underline{x}_i)^{-2}.$$



$\Rightarrow$



- Linearizations of $\breve{q}(x)$ are easily updated after reducing the box $[\underline{x}, \bar{x}]$

Cuts for the Linear Relaxation

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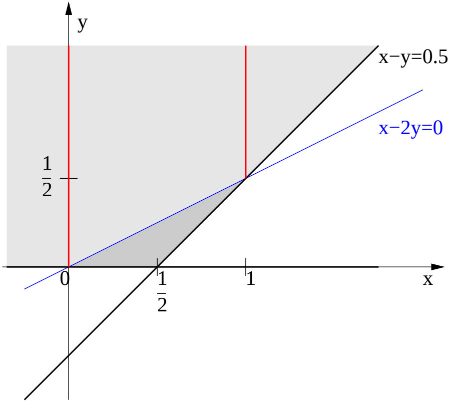
Mixed Integer Rounding Cut
(Nemhauser, Wolsey 1988) principle:

$$X := \{(x, y) \in \mathbb{Z} \times \mathbb{R}_+ \,|\, x - y \leq b\}$$

$$x - \frac{1}{1 - (b - \lfloor b \rfloor)} y \leq \lfloor b \rfloor \quad \forall (x, y) \in X$$



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Boxreduction based on intervalarithmetic

- Consider a constraint

$$g(x,y) := h(x) + y \leq 0,$$

i.e., $y \leq -h(x)$, and let

$$\left[\underline{h}, \bar{h}\right] := -h\left(\left[\underline{x}, \bar{x}\right]\right).$$

- If $\bar{h} \leq \bar{y}$, set

$$\bar{y} := \bar{h}$$

and proceed with other constraints depending on y.

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and proceed with other constraints depending on y.

- Does not rely on relaxations.
- Easy and fast to compute (GAMS-interface and FILIB++).
- Only one constraint at a time.

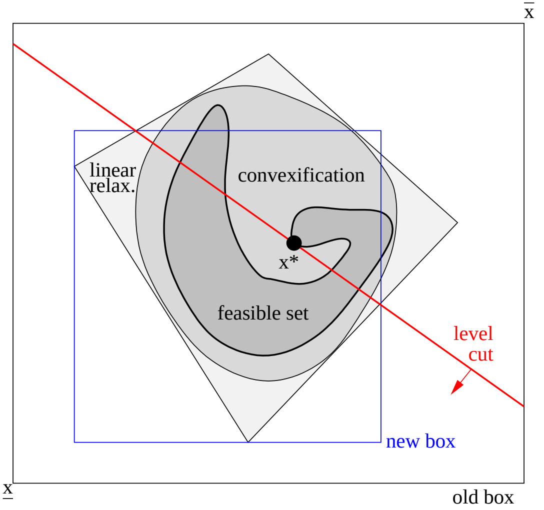
Boxreduction by enclosing the linear relaxation

Consider a linear relaxation with constraints $Ax \leq b$.

Let x^* be the best solution found so far.

$$\underline{x}_i := \min x_i \quad \text{s.t. } Ax \leq b, \quad c^T x \leq c^T x^*$$

$$\overline{x}_i := \max x_i \quad \text{s.t. } Ax \leq b, \quad c^T x \leq c^T x^*$$



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GAMS MINLPLib and GlobalLib

- at most 1000 variables and no integrality conditions except for binary
  $\Rightarrow$ 33 MIQQPs, 72 (nonquadratic) MINLPs, 163 QQPs
- timelimit: 1 hour
- NLP subsolver: CONOPT; LP subsolver: CPLEX 10.0

	MIQQPs	MINLPs
number of models	33	72
best known optimal solution found	21	42
local optimal solution found	4	10
no feasible point found	8	20

Pentium IV 3.00 Ghz, 1 GB RAM, Linux 2.16.11

LaGO vs. BARON on MIQQPs

LaGO and BARON 7.5 on MIQQPs from MINLPLib:

	Total	optimal value: LaGO better	optimal value: same	optimal value: BARON better
BARON fail, LaGO not	2	2		
LaGO faster	1		1	
both solvers the same	7		5	2
BARON faster	15	2	11	2
LaGO fail, BARON not	2			2
LaGO and BARON fail	6		6	
Total	33	4	23	6

convex MIQQPs: 5

LaGO vs. BARON on MINLPs

LaGO and BARON 7.5 on (nonquadratic) MINLPs from MINLPLib:

	Total	optimal value: LaGO better	same	BARON better
BARON fail, LaGO not	4	4		
LaGO faster	6	1	2	3
both solvers the same	7	1	5	1
BARON faster	35	4	25	6
LaGO fail, BARON not	8			8
LaGO and BARON fail	12		12	
Total	72	10	44	18

convex MINLPs: 20

LaGO stops branching when all binary variables are fixed (due to missing update of quadratic underestimators)

LaGO vs. BARON on QQPs

running LaGO and BARON 7.5 on QQPs from GlobalLib:

	Total	optimal value		
		LaGO better	same	BARON better
BARON fail, LaGO not	1	1		
LaGO faster	13	1	12	
both solvers the same	82		81	1
BARON faster	65		65	
LaGO fail, BARON not	2			2
Total	163	2	158	3

convex QQPs: 12

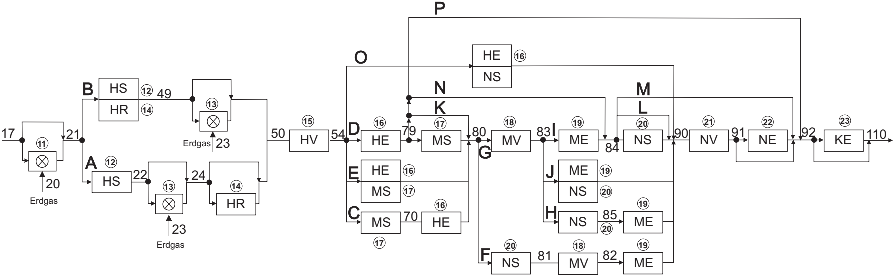
Optimizing the design of a complex energy conversion plant

2001-2004: project funded by German Science Foundation

Institute for Energy Engineering
(Technical University Berlin)
T. Ahadi-Oskui, F. Cziesla, G. Tsatsaronis

Institute for Mathematics
(Humboldt University Berlin)
H. Alperin, I. Nowak, S. Vigerske

- Model: superstructure of a combined-cycle-based cogeneration plant
- Simultaneous structural and process variable optimization



picture: exhaust gas path through heat-recovery steam generator

Model of a complex energy conversion plant

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  - purchase equipment costs
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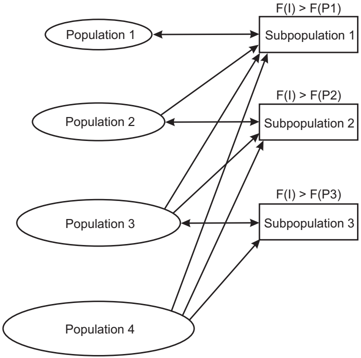
- MINLP model:
  - 1308 variables (44 binary, 3%)
  - 1659 constraints (376 nonlinear, 23%)
  - maximal block size: 6
  - quadratic underestimators computed: 329
- GAMS MINLPLib models super1, super2, super3, and super3t

Distributed genetic algorithm

- individual = set of decision variables
- fitness obtained by simulation of the superstructure

HSC-GA: hierarchical social competition algorithm:

- handling several populations in parallel
- organized by fitness of inhabitants
- individuals from lower population can move into subpopulation at higher level
- after evolving for some time, they migrate into higher population



Optimization of the superstructure

- HSC-GA and LaGO run for 24 hours
  - HSC-GA: ≈ 20000 generations
  - LaGO: ≈ 30000 Branch and Bound iterations

demand	method	efficiency	cost
electric power: 300 MW	LaGO	56.7%	12674 Euro/h
	HSC-GA	55.4%	12774 Euro/h
electric power: 290 MW	LaGO	68.5%	13424 Euro/h
process steam: 150 t/h	HSC-GA	67.7%	13399 Euro/h
electric power: 400 MW	LaGO	58.6%	16771 Euro/h
	HSC-GA	58.7%	17229 Euro/h

Turang Ahadi-Oskui (2006): Optimierung des Entwurfs komplexer Energieumwandlungsanlagen, Fortschritts-Berichte VDI, Reihe 6, Nr. 543.

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Intervalgradient Cuts

- Replace linear relaxation by a mixed-integer linear relaxation.

Allows use of intervalgradient cuts (Boddy and Johnson 2003 for MIQQPs):

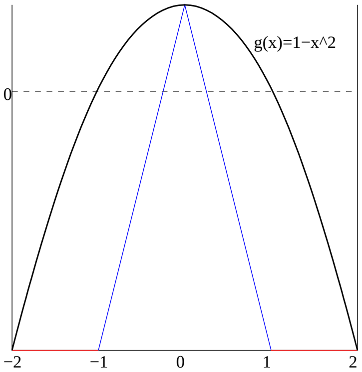
Intervalgradient of $g(x)$:

$$\left[\underline{d}, \bar{d}\right] := \nabla g\left([\underline{x}, \bar{x}]\right)$$

Intervalgradient cut w.r.t. $\hat{x} \in [\underline{x}, \bar{x}]$:

$$g(\hat{x}) + \min_{d \in [\underline{d}, \bar{d}]} d^T (x - \hat{x}) \leq 0$$

- better approximation of nonconvexities
- local exact ⇒ finite convergence
- independent of relaxations



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many things to improve, e.g.,

- support of integer variables
- branching rules
- node selection rules
- generation of quadratic underestimators during Branch and Bound
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