LaGO

a Branch and Cut framework for nonconvex MINLPs

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Lagrangian Global Optimizer

General purpose solver for sparse, block-separable, nonconvex MINLPs

History:

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

- Branch and Cut for MIQQPs
- heuristic Branch and Cut for nonconvex MINLPs
- start of Branch Cut and Price algorithm for MINLPs

Webpage: `http://www.math.hu-berlin.de/~eopt/LaGO`

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

Overview

MINLP

We consider problems of the form

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

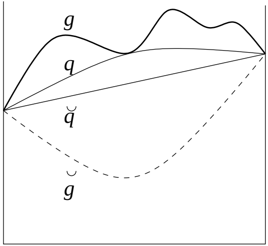
$-\infty < \underline{x}_i \leq \bar{x}^i < \infty$, $i \in \{1, \ldots, n\}$, $h \in C^2\left([\underline{x}, \bar{x}], \mathbb{R}^{|I|+|E|}\right)$, $c \in \mathbb{R}^n$

LaGO interfaces problems via GAMS

Overview

Preprocessing

- Investigation of problem structure (sparsity, block-separability, quadratic functions, convexity).
- Reduction of box $[\underline{x}, \bar{x}]$, determine bounding box for unbounded variables
- Initialization of linear relaxation:
  1. Nonquadratic nonconvex function g
     $\Rightarrow$ quadratic (nonconvex) underestimator q
  2. Quadratic nonconvex function q
     $\Rightarrow$ quadratic convex underestimator $\breve{q}$
  3. Nonlinear convex function $\Rightarrow$ linearization
  4. Binary conditions are dropped.



Nonconvex quadratic underestimator

Let $g \in C^2([\underline{x}, \bar{x}], \mathbb{R})$ be nonquadratic. Consider a sample set $S \subseteq [\underline{x}, \bar{x}]$.

We compute $q(x) = x^T A x + b^T x + c$ by minimization of

$$\sum_{x \in S} (g(x) - q(x)) + \delta_1 \sum_{x \in S_1} |\nabla (g - q)(x)|_1 + \delta_2 \sum_{x \in S_2} \left|\nabla^2 (g - q)(x)\right|_1$$

such that $q(x) \leq g(x)$ for all $x \in S$, where $S_2 \subseteq S_1 \subseteq S$ and $\delta_1, \delta_2 \geq 0$.

- Can be formulated as a linear program.
- Sparsity of A and b determined by $g(x)$.

Convex quadratic underestimator

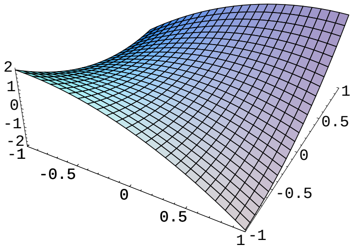
Let $q(x) = x^T A x + b^T x + c$ be a quadratic nonconvex function.

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

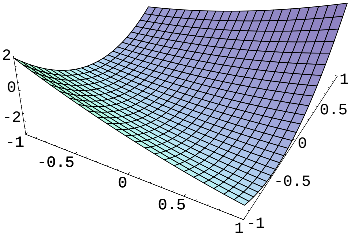
$$\breve{q}(x) = q(x) + \sum_{i=1}^{n} \alpha_i (x_i - \underline{x}_i)(x_i - \bar{x}_i)$$

where

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



$\Longrightarrow$



Overview

Main Loop

Denote by $\hat{x}$ a solution of the linear relaxation.

1. Take node with lowest lower bound from Branch and Bound tree.
2. Upper bounds: Start local search (with fixed binary variables) from $\hat{x}$ (rounded) (GAMS/NLP-Solver or IPOPT)

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3. Branch: select a variable x_i
   - whose binary condition is mostly violated by $\hat{x}$
   - or: where $g(x) \leq 0$ is mostly violated by $\hat{x}$, $\frac{\partial}{\partial x_i} g(\hat{x})$ is large, and the box of x_i hasn't been reduced very much so far
   - or: whose box is least reduced

Main Loop

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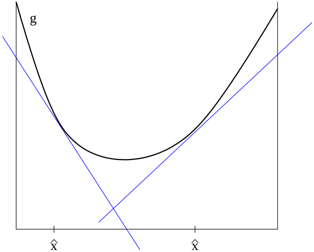
   - or: whose box is least reduced
4. Bound: for each child node
   - 4.1 Generate and update cuts
   - 4.2 Update the box
   - 4.3 Solve the linear relaxation (CPLEX or COIN/Clp)
   - 4.4 Put nodes into tree
5. Prune: Prune nodes which lower bound exceeds upper bound

Overview

Linearization Cuts

reference point $\hat{x}$, convex constraint $g(x) \leq 0$

$$g(\hat{x}) + \nabla g(\hat{x})(x - \hat{x}) \leq 0$$



Linearizations of convexified functions

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

can easily be updated after a reduction of the box $[\underline{x}, \bar{x}]$.

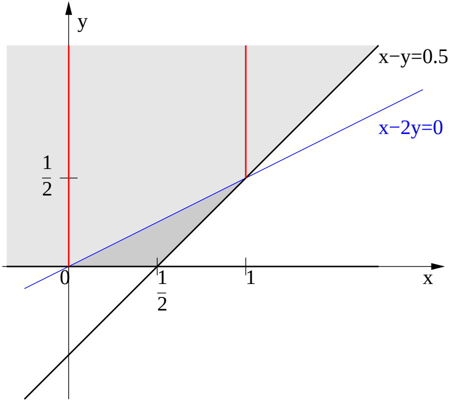
Mixed Integer Rounding Cuts

- Linear relaxation solved via COIN Open Solver Interface
- COIN Cut Generator Library provides several types of cuts to cut off a nonintegral solution of the relaxation

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

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

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



Overview

Boxreduction based on intervalarithmetic

- Consider a constraint

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

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

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

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

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

and proceed with other constraints depending on y.
- Does not rely on relaxations. Easy and fast to compute.
- Interval arithmetic provided by GAMS-interface and FILIB++.

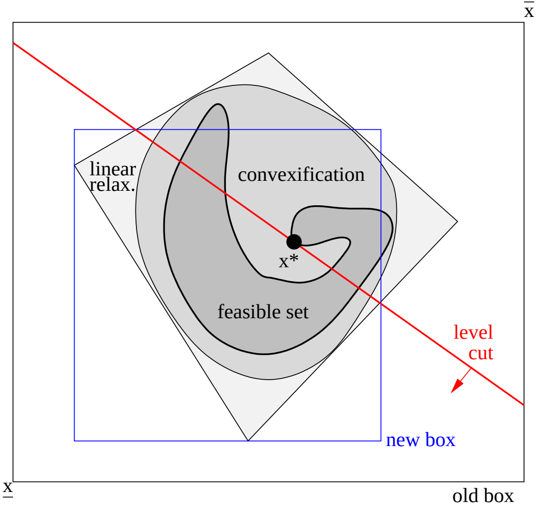
Boxreduction based on linear relaxation

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

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

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

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



Overview

GAMS MINLPLib and GlobalLib

- at most 1000 variables and no integrality conditions except for binary
  $\Rightarrow$ 33 MIQQPs, 72 (nonquadratic) MINLPs, 166 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	41
nonoptimal solution found	5	9
unsuccessful Branch & Cut search	7	13
failure in preprocessing	0	9

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	3	3		
LaGO faster	1		1	2
both solvers the same	7		5	
BARON faster	15	2	12	1
LaGO fail, BARON not	2			2
LaGO and BARON fail	5		5	
Total	33	5	23	5

LaGO vs. BARON on MINLPs

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

		optimal value		
	Total	LaGO better	same	BARON better
BARON fail, LaGO not	5	5		
LaGO faster	10	1	4	5
both solvers the same	10	1	9	
BARON faster	25	3	18	4
LaGO fail, BARON not	11			11
LaGO and BARON fail	11		11	
Total	72	10	38	20

LaGO stops branching when all binary variables are fixed

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	11	1	9	1
both solvers the same	90		89	1
BARON faster	61		61	
LaGO fail, BARON not	3			3
Total	166	2	159	5

Optimizing the design of a complex energy conversion plant

2001-2004: project funded by German Science Foundation

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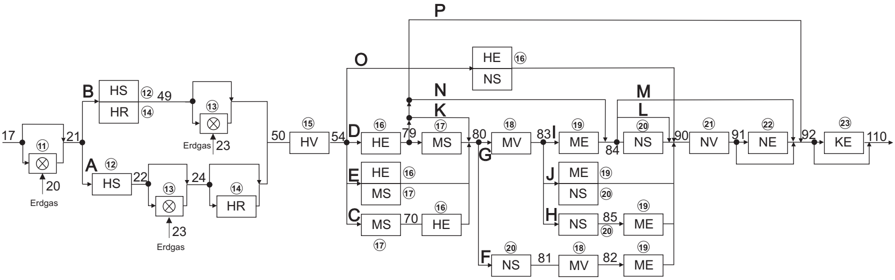
H. Alperin, I. Nowak, S. Vigerske

- 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

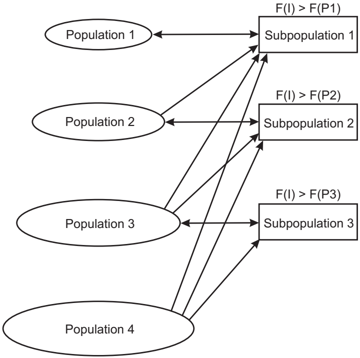
- superstructure for electric power output of ≤ 400 MW and process steam production of ≤ 500 t/h
- degrees of freedom: 27 structural and 48 process variables
- constraints:
  - logic of the superstructure (connecting binary variables)
  - thermodynamic behavior (highly nonlinear), mass+energy balances
  - purchase equipment costs
- objective: total cost for cogeneration plant
  investment cost, operation and maintenance cost, taxes and insurances,...
- MINLP model: 1308 variables (44 binary) and 1659 constraints
- 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: $\approx$ 20000 generations
  - LaGO: $\approx$ 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 process steam: 150 t/h	LaGO	68.5%	13424 Euro/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.

Overview

Mixed-integer linear relaxation

- MIP solver are fast and robust today.
- Replace linear relaxation by a mixed-integer linear relaxation.

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

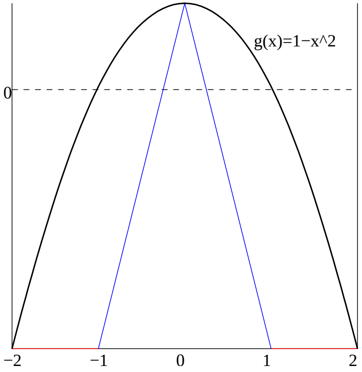
Intervalgradient of g:

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

$\left(\nabla g(x) \in \left[\underline{d}, \bar{d}\right] \; \forall x \in [\underline{x}, \bar{x}]\right)$

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

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



Intervalgradient Cuts

Intervalgradient cut w.r.t. $\hat{x} \in [\underline{x}, \bar{x}]$: $\left[\underline{d}, \bar{d}\right] := \nabla g\left([\underline{x}, \bar{x}]\right)$

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

Reformulation:

$$\begin{aligned}
g\left(\hat{x}\right) + \underline{d}^T y^+ - \bar{d}^T y^- &\leq 0 \\
x - \hat{x} &= y^+ - y^- \\
0 \leq y_i^+ &\leq z_i\left(\bar{x}_i - \hat{x}_i\right), \qquad i = 1, \ldots, n \\
0 \leq y_i^- &\leq \left(1 - z_i\right)\left(\hat{x}_i - \underline{x}_i\right), \quad i = 1, \ldots, n \\
& z_i \in \{0, 1\}, \qquad i = 1, \ldots, n
\end{aligned}$$

- applied to original formulation of MINLP, independent of relaxations
- currently implemented in LaGO with relaxed binary conditions

Further improvements...

- reliable underestimators of nonquadratic nonconvex functions
- support of integer variables
- branching rules
- node selection rules
- ...

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Thank you!

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