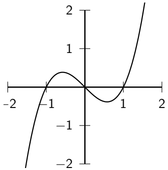
Pierre Bonami
IBM ILOG CPLEX
CO@Work - ZIB - October 7 2015

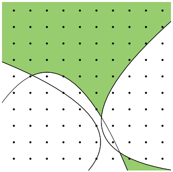
Algorithms for Mixed Integer Nonlinear Optimization

Introduction

The mother of all deterministic optimization problems [Lee, 2008]

$$
\begin{array}{lll}
\min & f(x) & \\
\text{s.t.} & g_i(x) \leq 0 & i = 1, \ldots, m \\
& x \in X & \\
& x_j \in \mathbb{Z} & j = 1, \ldots, p \\
& l_j \leq x_j \leq u_j & j = 1, \ldots, p
\end{array}
\qquad \text{(MINLP)}
$$



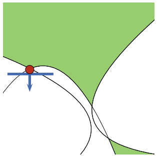


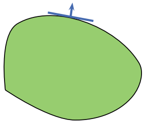
- $X \subseteq \mathbb{R}^n$ polyhedral.
- f and $g_i : X \to \mathbb{R}$, $i = 1, \ldots, m$, continuous, differentiable.

"Well solved" subproblems

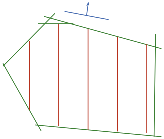
Nonlinear Programming (NLP)

$p = 0$: local optima. $\quad + f$ and g_i convex $\Rightarrow$ global optima.





Mixed-Integer linear programming (MILP)



- f linear, $m = 0$, $p > 0$

The complexity issue

Theorem ([Jeroslow, 1973])

The problem of minimizing a linear form over quadratic constraints in integer variables is not computable by a recursive function.

Theorem ([De Loera et al., 2006])

The problem of minimizing a linear function over polynomial constraints in at most 10 integer variables is not computable by a recursive function.

The complexity issue

There is no algorithm to solve (MINLP) ...

Theo

The p minimizing a linear form over quadratic constraints in integer variables is not computable by a recursive function.

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The complexity issue

There is no algorithm to solve (MINLP) …

Theo

The p … minimizing a linear form over quadratic constraints in integer variables is not computable by a recursive function.

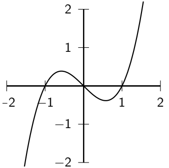
Theorem ([De Loera …

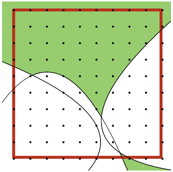
… even with 10 variables.

The p … over polynomial constraints in at most … not computable by a recursive function.

MINLP

$$
\begin{array}{lll}
\min & f(x) & \\
\text{s.t.} & g_i(x) \le 0 & i = 1, \ldots, m \\
 & x \in X & \\
 & x_j \in \mathbb{Z} & j = 1, \ldots, p \\
 & l_j \le x_j \le u_j & j = 1, \ldots, p
\end{array}
\qquad \text{(PNLM)}
$$





- **To be solvable in general, l_j, u_j finite.**

Two main classes of MINLP

Mixed Integer Convex Program

Assume that the continuous relaxation is a convex optimization problem.

- f is a convex function.
- g_i are convex functions.

Mixed Integer Nonlinear Program (or Global Optimization)

Don't assume any convexity on f or g_i.

- Continuous relaxation is NP-hard to solve in general.
- Remark: if l_j and u_j are finite integers, variable x_j can be seen as a continuous variable satisfying:

$$(x_j - l_j)(x_j - l_j - 1)....(x_j - u_j) = 0$$

A special class of convex MINLP: MISOCP

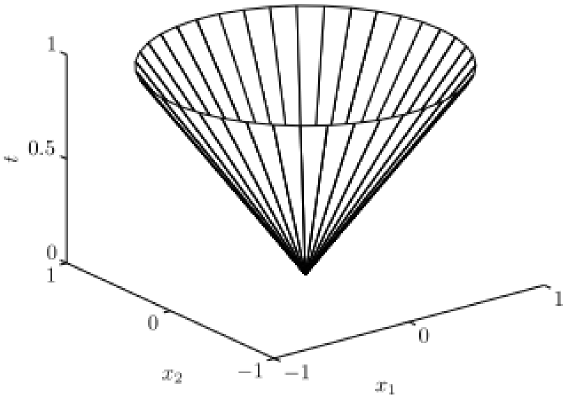
$$\begin{array}{lll} \min & c^T x & \\ & x^T Q_k x + a_k^T x \leq a_k^0 & k = 1, \ldots, m, \\ & Ax = b, & \\ & x_j \in \mathbb{Z} & j = 1, \ldots, p. \end{array} \qquad \text{(MIQCP)}$$

Where all quadratic constraints can be represented as second order cones (or Lorentz cone):

$$L^d := \{(x, x_0) \in \mathbb{R}^{d+1} : \sum_{i=1}^{d} x_i^2 \leq x_0^2, x_0 \geq 0\}.$$

(L^d defines the $(d+1)$-dimensional second order cone.)

A Lorentz cone



It is convex!

Second order cone representability

Through simple algebra can be represented as second order cones:

- Second order cones: $\sum_{i=1}^{d} x_i^2 \leq x_0^2$, with $x_0 \geq 0$
- Rotated second order cones: $\sum_{i=2}^{d} x_i^2 \leq x_0 x_1$, with $x_0, x_1 \geq 0$
- Simple convex quadratic constraints:

$$x^T Q x + a^T x \leq a^0, \text{ with } Q \succeq 0$$

- or more complicated...

$$||x^T Q x + a^T x|| \leq c^T x + b, \text{ with } Q \succeq 0$$

(the first three should be recognized by most solvers, the last one not.)

Many non-linear constraints can be formulated as second order cones but modeling may be very far from obvious.

MISOCP

$$
\begin{aligned}
\min \quad & c^T x \\
& (x_{J_i}, x_{h_i}) \in L^{d_i} \quad & i = 1, \ldots, m \\
& Ax = b, \\
& x_j \in \mathbb{Z} & j = 1, \ldots, p.
\end{aligned}
\tag{MISOCP}
$$

MINLP's where all nonlinear constraints are SOC

- Continuous relaxation solved efficiently by interior points.
- convex MINLP algorithms work with some added technicality due to non-differentiability [Drewes, 2009, Drewes and Ulbrich, 2012].
- Supported by most MIP solvers (all the ones you saw these 2 weeks).

MISOCP Applications

Application	SOC	Integer
Portfolio optimization	Risk, utility, robustness	number of assets, min investment
[Bienstock, 1996, Bonami and Lejeune, 2009, Vielma et al., 2008]		
Truss topology optimization	Physical forces	Cross section of bars
[Achtziger and Stolpe, 2006]		
Networks with delays	Delay as function of traffic	Path, flows
[Boorstyn and Frank, 1977, Ameur and Ouorou, 2006]		
Location with stochastic services	Demands	location model
[Elhedhli, 2006]		
TSP with neighborhoods (Robotics)	Definition of ngbh.	TSP
[Gentilini et al., 2013]		
Many more... see for eg. http://cblib.zib.de.		

Mixed Integer Convex Programming Applications (not MISOCP)

Application	nonlinear	discrete
Chemical plant design	Chemical reactions	what to install
[Duran and Grossmann, 1986, Flores-Tlacuahuac and Biegler, 2007]		
Block Layout Design	Spatial constraints	what to layout
[Castillo et al., 2005]		

Mixed Integer Nonlinear Programming Applications

Application	nonlinear	discrete
Petrochemical [Haverly, 1978]	Blending, pooling	–
Gaz/Water networks [Koch et al., 2015, Bragalli et al., 2011]	you know from	last week
Nuclear Reactor reloading [Quist et al., 1999]	reactions	What to reload
Airplane trajectories [Cafieri and Durand, 2013, Soler et al., 2013]	aerodynamics	waypoints, colisions
Mixed Integer Optimal control [Sager, 2005, 2012]	DE	discrete controls
Countless more see for example [Belotti et al., 2013b]	...	...

Agenda

- Part I: The Basic Algorithms.
  - The Convex Case
    - Main Algorithmic Approaches
    - Glimpse of Computations
    - Glimpse of MISOCP
  - Steps into Non-Convexity.
    - Non-convex MIQP
    - Basic Setup of a Spatial Branch-and-Bound.
    - Generalizing.
    - Glimpse of solvers, Libraries, Performance: S. Vigerske.
- Part II: Selected Advanced (or not) Topics.
  - A most simple MINLP.
  - MILP vs. Non-Convex QPs.
  - Everything can go wrong easily.

Part I

The Basic Algorithms

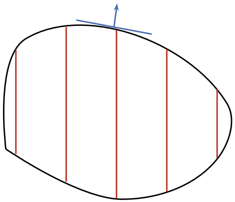
The Basic Algorithms

Section 1

The convex case

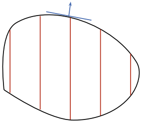
The mixed integer convex program

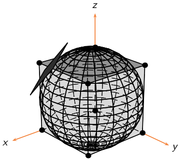
$$
\begin{array}{lll}
\min & c^T x & \\
\text{s.t.} & g_i(x) \leq 0 & i = 1, \ldots, m \\
 & x \in X & \\
 & x_j \in \mathbb{Z} & j = 1, \ldots, p
\end{array}
\qquad \text{(MICP)}
$$



- $g_i : X \to \mathbb{R}$, $i = 1, \ldots, m$, convex, differentiable.
- Assume linear objective. If necessary, add var $\alpha \in \mathbb{R}$ and $\min \alpha$ with $f(x) \leq \alpha$ a constraint.

Main Algorithms for solving (MICP)





Fundamental property is convexity of the continuous relaxation, which can be efficiently solved.

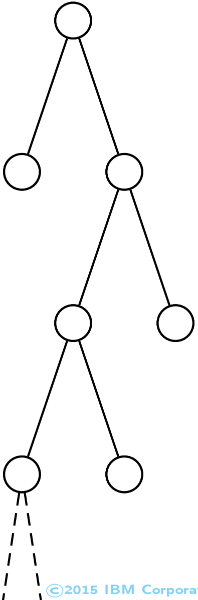
1. NLP Branch-and-bound [Gupta and Ravindran, 1985].
2. Outer Approximation Algorithm [Duran and Grossmann, 1986]. Builds an MILP equivalent of (MICP)
3. LP/NLP branch-and-cut [Quesada and Grossmann, 1992].

NLP based branch-and-bound

Straightforward generalization of main MILP algorithm:

- solve an NLP at each node of the tree.

NLP based branch-and-bound



Straightforward generalization of main MILP algorithm:

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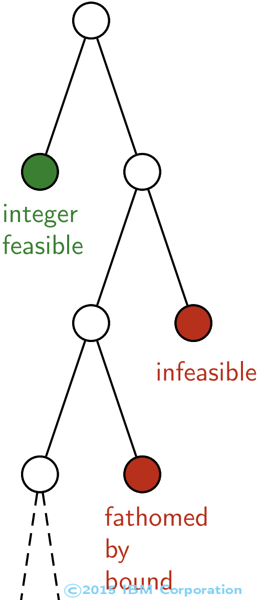
- Branch on variables with fractional value.

NLP based branch-and-bound

Straightforward generalization of main MILP algorithm:

- solve an NLP at each node of the tree.
- Branch on variables with fractional value.
- Prune by infeasibility, bounds and integer feasibility.



NLP based branch-and-bound

Straightforward generalization of main MILP algorithm:

- solve an NLP at each node of the tree.
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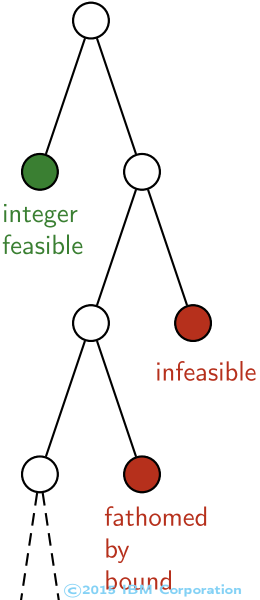
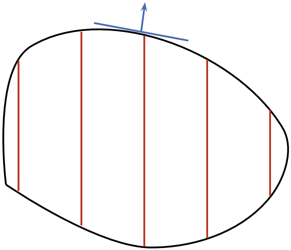
Main issues

- Warm-starting of NLP solves.
- Stability of NLP solvers.
- Difficulty of reusing MILP technologies.



Outer Approximation [Duran and Grossmann, 1986]



$$
\begin{aligned}
&\min \quad c^T x \\
&\text{s.t.} \\
&g_i(x) \le 0 \qquad i = 1, \dots, m, \\
&x_j \in \mathbb{Z}, \qquad j = 1, \dots, p.
\end{aligned}
$$

Idea: Take first-order approximations of constraints at different points and build an equivalent MILP.

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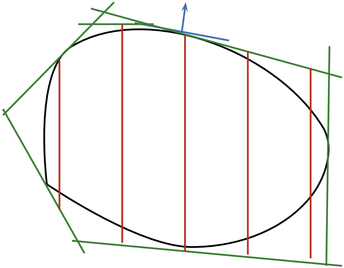

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Idea: Take first-order approximations of constraints at different points and build an equivalent MILP.

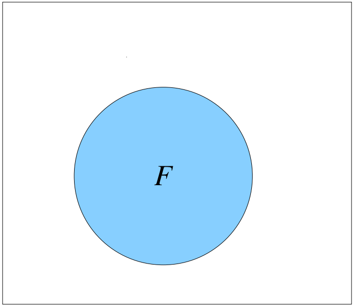
$$\begin{aligned} &\min \quad c^T x \\ &\text{s.t.} \\ &g_i(\bar{x}^k) + \nabla g_i(\bar{x}^k)^T (x - \bar{x}^k) \le 0 \qquad i = 1, \dots, m,\ k = 1, \dots, K \\ &x_j \in \mathbb{Z}, \qquad\qquad j = 1, \dots, p. \end{aligned}$$

Outer approximation constraints

Let $F := \{x : x \in X : g_i(x) \leq 0\}$
$(g_i : \mathbb{R}^n \to \mathbb{R}$ convex. $)$
Outer approximation constraint in $\bar{x}$:

$$\nabla g_j(\bar{x})^T (x - \bar{x}) + g_j(\bar{x}) \leq g_j(x) \leq 0.$$

(valid for F by convexity of g_j and definition of F.)



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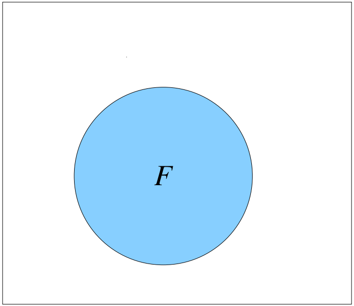

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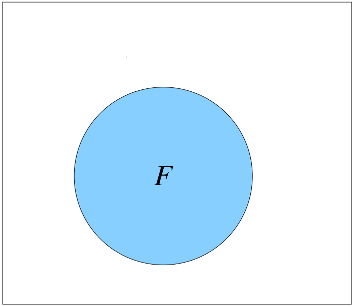

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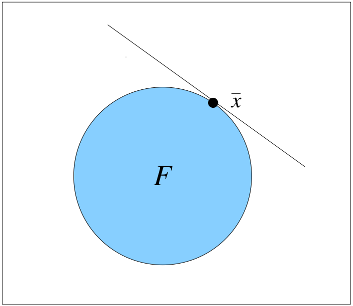
(valid for F by convexity of g_j and definition of F.)

- If $g(\bar{x}) = 0$ tangent to feasible region.
- If $g(\bar{x}) < 0$ non-tight constraint.
- If $g(\bar{x}) > 0$ non-tight constraint cutting off $\bar{x}$.



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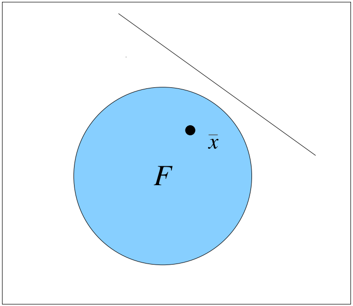

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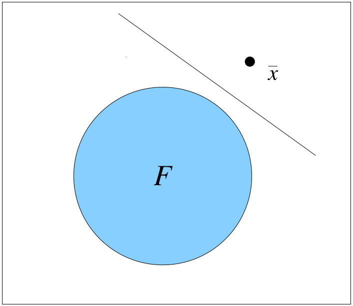


Subproblems

Given $\hat{x} \in \mathbb{R}^p$:

fixed NLP (NLP($\hat{x}$))

$$
\begin{aligned}
& \min\ c^T x \\
& s.t. \\
& g_i(x) \leq 0, && i = 1, \dots, m \\
& x \in X; && \text{(NLP}(\hat{x})) \\
& x_j = \hat{x}_j, && j = 1, \dots, p.
\end{aligned}
$$

If $\hat{x} \in \mathbb{Z}^p$, and feasible: gives an upper bound.

fixed feasibility subproblem

$$
\begin{aligned}
& \min \sum_{i=1}^{m} w_i \max\{0, g_i(x)\} \\
& \text{s.t.} \\
& x \in X, && \text{(NLPF}(\hat{x})) \\
& x_j = \hat{x}_j,\ j = 1, \dots, p
\end{aligned}
$$

Subproblems

Given $\hat{x} \in \mathbb{R}^p$:

fixed NLP (NLP($\hat{x}$))

$$\begin{aligned} & \min\ c^T x \\ & s.t. \\ & g_i(x) \leq 0, \qquad i = 1, \ldots, m \\ & x \in X; \qquad\qquad (\text{NLP}(\hat{x})) \\ & x_j = \hat{x}_j, \qquad j = 1, \ldots, p. \end{aligned}$$

If $\hat{x} \in \mathbb{Z}^p$, and feasible: gives an upper bound.

fixed feasibility subproblem

$$\begin{aligned} & \min \sum_{i=1}^{m} w_i \max\{0, g_i(x)\} \\ & \text{s.t.} \\ & x \in X, \qquad\qquad (\text{NLPF}(\hat{x})) \\ & x_j = \hat{x}_j,\ j = 1, \ldots, p \end{aligned}$$

Remark If (NLP($\hat{x}$)) is infeasible, NLP software will typically return a solution to (NLPF($\hat{x}$)). By abuse, always say solution to (NLP($\hat{x}$))

Equivalent MILP formulation of convex MINLP

For each $\hat{x}^k \in K = \mathrm{Proj}_{1,\ldots,p}(X) \cap \mathbb{Z}^p$, let $\overline{x}^k$ be an optimal solution to (NLP($\hat{x}$)).

Theorem ([Duran and Grossmann, 1986])

If $X \neq \emptyset$, f and g are convex, continuously differentiable, and a constraint qualification holds for each $\overline{x}^k$ then

$$
\begin{aligned}
&\min \quad c^T x \\
&g_i(\overline{x}^k) + \nabla g_i(\overline{x}^k)^T (x - \overline{x}^k) \leq 0 \quad i = 1, \ldots, m, \hat{x}^k \in K, \\
&x \in X,\ x_j \in \mathbb{Z},\ j = 1, \ldots, p.
\end{aligned}
$$

has the same optimal value as (MICP).

OA decomposition

Generate MILP equivalent by constraint generation.

- Initialize with one set of linearizations.

$$
\begin{aligned}
\min \quad & c^T x \\
\text{s.t.} \quad & \\
& g_i(\bar{x}^0) + \nabla g_i(\bar{x}^0)^T (x - \bar{x}^0) \le 0, \qquad i = 1, \ldots, m, \quad , \\
& x \in X,\ x_j \in \mathbb{Z},\ j = 1, \ldots, p.
\end{aligned}
\tag{OA($\mathcal{K}$)}
$$

Where x^0 is the solution to the continuous relaxation:
$\min\{c^T x : x \in X,\ g_i(x) \le 0, i = 1, \ldots, m\}$

OA decomposition

Generate MILP equivalent by constraint generation.

- Initialize with one set of linearizations.
- Enrich iteratively the set of linearizations $\mathcal{K}$.

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & \\ & g_i(\overline{x}^k) + \nabla g_i(\overline{x}^k)^T (x - \overline{x}^k) \le 0, \qquad \begin{array}{c} i = 1, \ldots, m, \\ \hat{x}^k \in \mathcal{K} \end{array} , \\ & x \in X, \, x_j \in \mathbb{Z}, \, j = 1, \ldots, p. \end{aligned} \tag{OA($\mathcal{K}$)}$$

Where $\hat{x}^k$ is a solution to (OA($\mathcal{K}$)) and, for $k = 1, \ldots, |\mathcal{K}|$, $\overline{x}^k$ is the solution to (NLP($\hat{x}$)).

OA decomposition

Generate MILP equivalent by constraint generation.

- Initialize with one set of linearizations.
- Enrich iteratively the set of linearizations $\mathcal{K}$.

Convergence

At each iteration:

- (OA($\mathcal{K}$)) gives a lower bound,
- If feasible, (NLP($\hat{x}$)) gives an upper bound.

The OA Theorem guarantees that the two bounds converge in finite # of iterations.

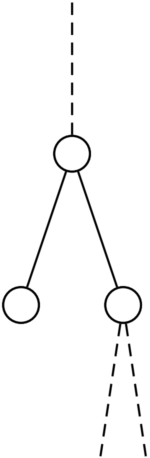
Outer-Approximation Decomposition Algorithm

0. **Initialize.**
   $z_U \leftarrow +\infty$. $z_L \leftarrow -\infty$. Let $\overline{x}^0$ be the optimal solution of continuous relaxation.
   $\mathcal{K} \leftarrow \left\{\overline{x}^0\right\}$. Choose a convergence tolerance ϵ.
1. **Terminate?**
   Is $z_U - z_L < \epsilon$ or (OA($\mathcal{K}$)) infeasible? If so z_U is $\epsilon-$optimal.
2. **Lower Bound**
   Let $z_{\mathrm{MP}(\mathcal{K})}$ be the optimal value of OA($\mathcal{K}$) and ($\hat{x}$) its optimal solution.
   $z_L \leftarrow z_{\mathrm{MP}(\mathcal{K})}$
3. **NLP Solve**
   Solve (NLP($\hat{x}$)).
   Let $\overline{x}^i$ be the optimal (or minimally infeasible) solution.
4. **Upper Bound?**
   Is $\overline{x}^i$ feasible for (MINLP)? If so, $z_U \leftarrow \min(z_U, f(\overline{x}^i))$.
5. **Refine**
   $\mathcal{K} \leftarrow \mathcal{K} \cup \{\overline{x}^i\}$ and $i \leftarrow i + 1$.
   Go to 1.

LP/NLP Branch-and-bound

OA can be embedded in a single tree search.

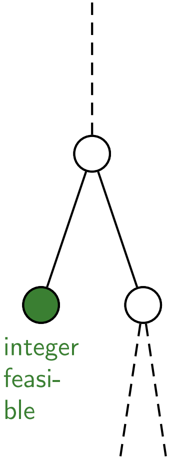
- Start solving the same initial MILP by branch-and-bound.
- At each integer feasible node:



LP/NLP Branch-and-bound

OA can be embedded in a single tree search.

- Start solving the same initial MILP by branch-and-bound.
- At each integer feasible node:
  1. solve (NLP($\hat{x}$)), and enrich the set of linearizations.
  2. Resolve the LP relaxation of the node with the new cuts.
  3. Repeat as long as node is integer feasible.



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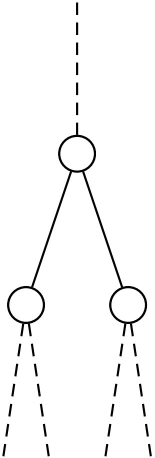

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- At each integer feasible node:
  1. solve (NLP($\hat{x}$)), and enrich the set of linearizations.
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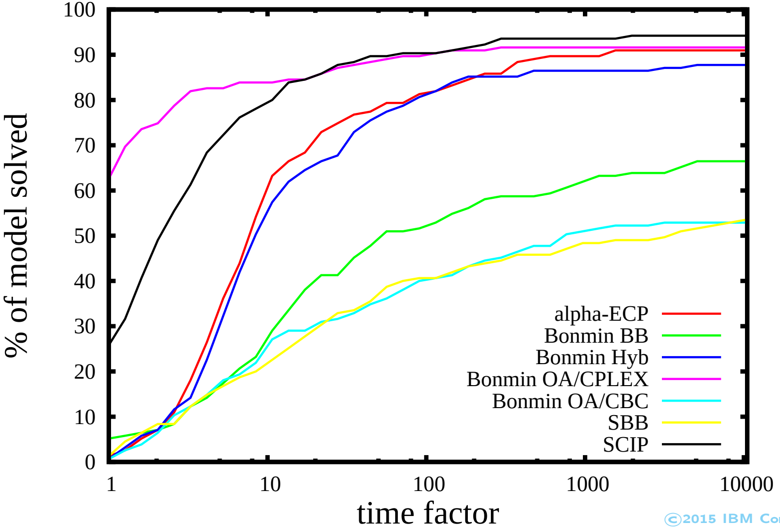
  3. Repeat as long as node is integer feasible.
- Never prune by integer feasibility.

Solvers for Mixed Integer Convex Programs

Solver	Reference	Algorithm(s)
Dicopt		OA
MINLP_BB	[Leyffer, 1998]	NLP BB
SBB	[Bussieck and Drud, 2001]	NLP BB
α-ECP	[Westerlund and Lundqvist, 2005]	ECP (variant of OA)
Bonmin	[Bonami et al., 2008]	NLP BB, OA, LP/NLP
FilMINT	[Abhishek et al., 2010]	LP/NLP
KNITRO	[Byrd et al., 2006]	NLP BB, LP/NLP
SCIP	[Vigerske, 2012]	LP/NLP

Comparison of solvers in GAMS [Vigerske, 2013]



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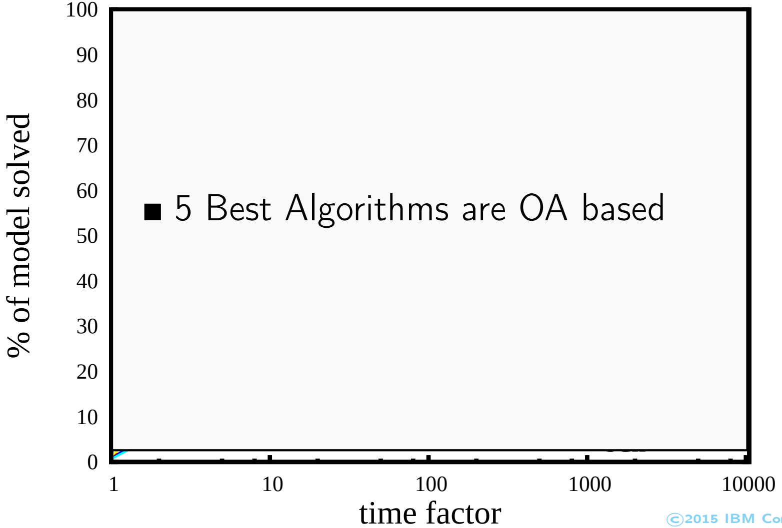

- 5 Best Algorithms are OA based

Notes on results with Bonmin

- Bonmin's OA using CPLEX seems the best algorithm overall.
  - It is also the simplest: a loop calling CPLEX (MILP) and Ipopt (NLP) alternatively as black boxes.
  - Improves with CPLEX.
- Bonmin's Hyb is in the pack of relatively good solvers
  - own variant of LP/NLP BB.
  - Reuse CBC infrastructure, LP solver, Cuts, MIP presolve.
  - Improves at a slower pace.
- Bonmin's BB clearly behind.
  - pure NLP based branch-and-bound. Doesn't reuse much from Cbc. Everything specifically tailored.
  - Better implementation exists that should be on par with Hyb.
- Bonmin's OA using CBC seems the worst algorithm overall.

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- Bonmin's OA using CBC seems the worst algorithm overall.

The MIQCP/MISOCP solver in CPLEX

Implements the two main algorithms:

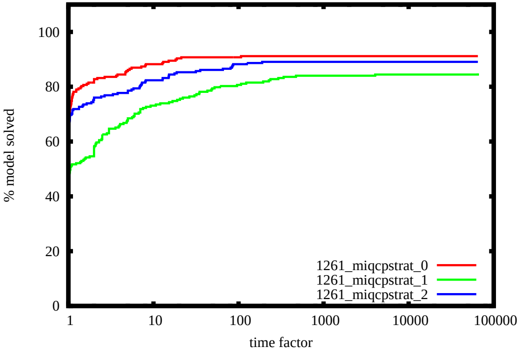
- A branch-and-bound based on the continuous SOCP solver (barrier).
- An outer approximation branch-and-cut algorithm.

Choice is controled by the parameter `CPXPARAM_MIP_Strategy_MIQCPStrat`.
Default is trying to decide which of the two algorithms to run in a "clever" way.

History of MIQCP with CPLEX

class	p	algorithm	V. (Year)
Convex QCP	0	barrier	9.0 (2003)
convex MIQCP	> 0	barrier based B&B	9.0 (2003)
–	–	Outer approximation B&C	11.0 (2007)

A comparison of OA and SOCP-BB in CPLEX 12.6.1 [1]



Default strategy picked

- OA 113 times
- SOCP-BB 46 times
- 56 models identical with both

To be perfect should have picked

- 14 more models with OA
- 36 more models with SOCP-BB

[1] 225 models solved by at least one method and failed by none.

Advanced algorithms for convex case (non exhaustive references)

- Preprocessing/Modeling:
  - separability [Hijazi et al., 14]
  - perspective formulations [Frangioni and Gentile, 2006, Günlük and Linderoth, 2008]
  - propagation [Vigerske, 2012]
- Node relaxations/Branching:
  - QP Delaxations in strong-branching [Bonami et al., 2013]
  - QP Divings [Mahajan et al., 2012]
- Primal Heuristics:
  - Feasibility Pumps [Bonami et al., 2009],
  - Undercover [Berthold and Gleixner, 2013]
- Cuts:
  - Disjunctive Cuts [Kılınc et al., 2011, Bonami, 2011].
  - Conic Cuts for Conic Crogramming [Andersen and Jensen, 2013, Belotti et al., 2013a, Kılınç-Karzan and Yıldız, 2015, Modaresi et al., 2015] (among others)

The Basic Algorithms

Section 2

Steps into non-convexity

(MI)QP

$$
\begin{aligned}
\min \quad & \frac{1}{2}x^T Qx + c^T x \\
s.t. \quad & \\
& Ax = b && && \text{(MIQP)} \\
& x_j \in \mathbb{Z} && j = 1, \ldots, p \\
& l \leq x \leq u
\end{aligned}
$$

(with Q symmetric),

(MI)QP

$$\begin{aligned} &\min \ \frac{1}{2}x^T Qx + c^T x \\ &s.t. \\ &\qquad Ax = b \\ &\qquad x_j \in \mathbb{Z} \qquad\qquad j = 1, \ldots, p \\ &\qquad l \leq x \leq u \end{aligned} \qquad\qquad \text{(MIQP)}$$

(with Q symmetric),

History of MIQP with CPLEX

class	p	Q	algorithm	V. (Year)
Convex QP	0	$\succeq 0$	barrier	4.0 (1995)
–	–	–	QP simplex	8.0 (2002)
convex MIQP	> 0	$\succeq 0$	B&B	8.0 (2002)
nonconvex QP	0	$\not\succeq 0$	barrier (local)	12.3 (2011)
–	–	–	spatial B&B (global)	12.6 (2013)
nonconvex MIQP	> 0	$\not\succeq 0$	spatial B&B (global)	12.6 (2013)

Example

Let $G = (N, E)$ be a graph and Q be the incidence matrix of G. The optimal value of:

$$\max \frac{1}{2} x^T Qx$$
$$s.t.$$
$$\sum x_j = 1$$
$$x \geq 0.$$

is $\frac{1}{2}\left(1 - \frac{1}{\chi(G)}\right)$ where $\chi(G)$ is the clique number of G [Motzkin and Straus, 1965],

- $\Rightarrow$ QP is NP-hard
- More generally QPs on the simplex (general Q) can be solved by a nonlinear maximum clique algorithm [Scozzari and Tardella, 2008].

Local solver of nonconvex QP in CPLEX

- Primal Dual Interior Point Algorithm.
- Solves to a *local optima*: there exists no better solution in a non-empty neigborhood.
- Not enabled by default, if Q is indefinite CPLEX will return `CPXERR_Q_NOT_POS_DEF`.
- Activated by setting the option `optimality target` to 2 (or `CPX_OPTIMALITYTARGET_FIRSTORDER`).
- Own implementation of indefinite factorization.

Global (MI)QP in CPLEX

- Activated by setting `optimality target` to 3 (or `CPX_OPTIMALITYTARGET_OPTIMALGLOBAL`).
- Note: previous versions could already solve some nonconvex MIQPs (pure 0-1 QPs, convex after presolve...)

Notes on complexity

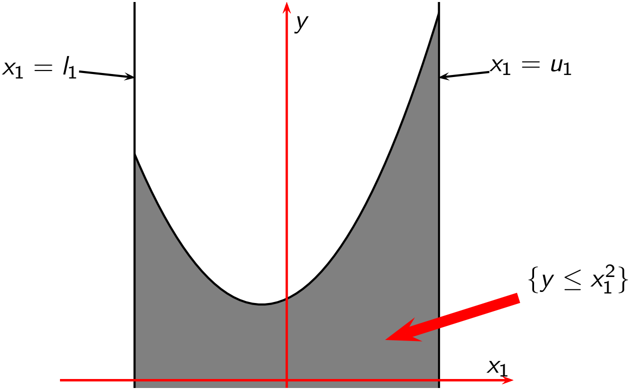
- Checking if a feasible solution is not a local minimum is coNP-Complete.
- Checking if a nonconvex QP is unbounded is NP-complete.

Spatial B&B

- Establish a convex (easily solvable) relaxation.
- Establish branching rules on solutions of this relaxation.

Elementary relaxations: Secant Approximation

The convex hull relaxations of a a square x_1^2



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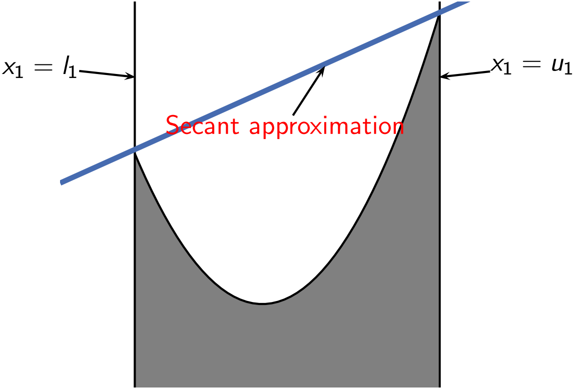

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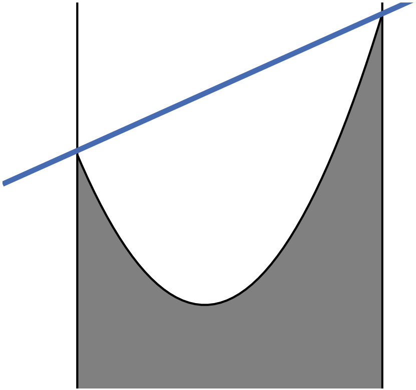
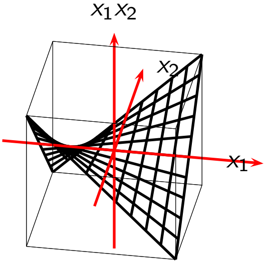


$$x_1^2 \leq y_{ii}^{+} := (l_1 + u_1)x_1 - l_1 u_1$$

Elementary relaxations: McCormick formulas

The convex hull relaxations of a single product $x_1 x_2$ [McCormick, 1976]

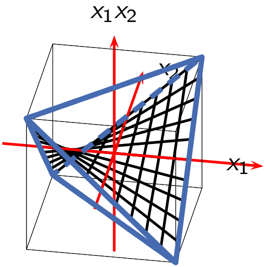


Elementary relaxations: McCormick formulas

The convex hull relaxations of a single product $x_1 x_2$ [McCormick, 1976]

$$x_1 x_2 \geq y_{12}^{-} := \max \left\{ \begin{array}{r} u_2 x_1 + u_1 x_2 - u_1 u_2 \\ l_2 x_1 + l_1 x_2 - l_1 l_2 \end{array} \right\}$$

$$x_1 x_2 \leq y_{12}^{+} := \min \left\{ \begin{array}{l} u_2 x_1 + l_1 x_2 - l_1 u_2 \\ l_2 x_1 + u_1 x_2 - u_1 l_2 \end{array} \right\}$$



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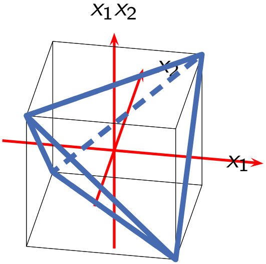


- Depending on the sign of q_{ij} we only need y^{+} or y^{-}.
- For simplicity, we assume we put all in the remainder.

Q-space reformulation and relaxation

- Let $Q = P + \tilde{Q}$ with P the diagonal psd matrix containing $q_{ii} > 0$.

$$
\begin{aligned}
& \min \ \frac{1}{2}x^T P x + \frac{1}{2}x^T \tilde{Q} x + c^T x \\
& s.t. \\
& Ax = b \\
& x_j \in \mathbb{Z} \qquad j = 1, \dots, p \\
& l \leq x \leq u
\end{aligned}
\qquad \text{(MIQP)}
$$

Q-space reformulation and relaxation

- Let $Q = P + \tilde{Q}$ with P the diagonal psd matrix containing $q_{ii} > 0$.
- Add one $y_{ij} = x_i x_j$ variable for each non-zero entry q_{ij} of $\tilde{Q}$.

$$
\begin{aligned}
& \min \ \frac{1}{2} x^T P x + \frac{1}{2} \langle \tilde{Q}, Y \rangle + c^T x \\
& s.t. \\
& Ax = b \\
& x_j \in \mathbb{Z} \qquad j = 1, \ldots, p \\
& Y = xx^T \\
& l \leq x \leq u
\end{aligned}
\qquad \text{(MIQP)}
$$

($\langle Q, Y \rangle = \sum_{i,j} q_{ij} y_{ij}$)

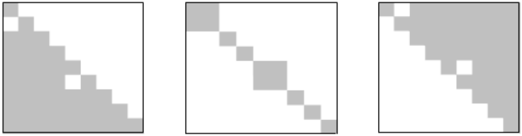
Q-space reformulation and relaxation

- Let $Q = P + \tilde{Q}$ with P the diagonal psd matrix containing $q_{ii} > 0$.
- Add one $y_{ij} = x_i x_j$ variable for each non-zero entry q_{ij} of $\tilde{Q}$.
- Relax $y_{ij} = x_i x_j$ using McCormick and Secant approximations.

$$
\begin{aligned}
& \min \ \frac{1}{2} x^T P x + \frac{1}{2} \langle \tilde{Q}, Y \rangle + c^T x \\
& s.t. \\
& Ax = b \\
& x_j \in \mathbb{Z} \qquad j = 1, \ldots, p \\
& y_{ij}^- \leq y_{ij} \leq y_{ij}^+ \\
& y_{ii} \leq y_{ii}^+ \\
& l \leq x \leq u
\end{aligned}
\tag{q-MIQP}
$$

Factorizations of Q

- Our block indefinite decomposition: M and B such that M 2-block triangular and B 2-blocks diagonal with $Q = M^T BM$



- Reformulate $x^T Qx$ using additional variables z so that $z^T Dz = x^T Bx$ and D diagonal. Let L, D give the spectral decomposition of B, $z = L\zeta$, $\zeta = Mx$.

(For simplicity assume $z = Lx$ gives the system we want)

Factorized Eigenvector space reformulation and relaxation

Use a decomposition to get $z = Lx$ and $z^T Dz = x^T Qx$ and do the same steps as before (but more simple)....

$$\begin{aligned}
&\min \ \frac{1}{2} z^T D z + c^T x \\
&s.t. \\
&Ax = b, Lx = z \\
&x_j \in \mathbb{Z} \qquad j = 1, \ldots, p \\
&l \leq x \leq u
\end{aligned} \tag{MIQP}$$

Factorized Eigenvector space reformulation and relaxation

Use a decomposition to get $z = Lx$ and $z^T Dz = x^T Qx$ and do the same steps as before (but more simple)....

- Let $D = D^+ - D^-$ with $D^\pm$ diagonal psd matrices.

$$
\begin{aligned}
& \min \ \frac{1}{2}(z^T D^+ z - z^T D^- z) + c^T x \\
& s.t. \\
& Ax = b, Lx = z \\
& x_j \in \mathbb{Z} \qquad\qquad j = 1, \ldots, p \\
& l \le x \le u
\end{aligned}
\qquad \text{(MIQP)}
$$

Factorized Eigenvector space reformulation and relaxation

Use a decomposition to get $z = Lx$ and $z^T Dz = x^T Qx$ and do the same steps as before (but more simple)....

- Let $D = D^+ - D^-$ with $D^\pm$ diagonal psd matrices.
- Add $y_{ii} \leq z^2$ variable for each non-zero of D^-.

$$
\begin{aligned}
\min \quad & \frac{1}{2} z^T D^+ z - \sum_{i=1}^{n} \frac{d_{ii}}{2} y_{ii} + c^T x \\
s.t. \quad & \\
& Ax = b, Lx = z \\
& x_j \in \mathbb{Z} \qquad\qquad j = 1, \ldots, p \\
& y_{ii} \leq z_i^2 \\
& l \leq x \leq u
\end{aligned}
\tag{MIQP}
$$

Factorized Eigenvector space reformulation and relaxation

Use a decomposition to get $z = Lx$ and $z^T D z = x^T Q x$ and do the same steps as before (but more simple)....

- Let $D = D^+ - D^-$ with $D^\pm$ diagonal psd matrices.
- Add $y_{ii} \leq z^2$ variable for each non-zero of D^-.
- Infer finite bounds, l^z, u^z for z and relax $y_{ii} \leq z_i^2$ using Secant approximations.

$$
\begin{aligned}
\min\ & \frac{1}{2} z^T D^+ z - \sum_{i=1}^{n} \frac{d_{ii}}{2} y_{ii} + c^T x \\
s.t.\ & \\
& Ax = b, Lx = z \\
& x_j \in \mathbb{Z} \qquad\qquad j = 1, \ldots, p \\
& y_{ii} \leq y_{ii}^+ \\
& l \leq x \leq u, l^z \leq z \leq u^z
\end{aligned}
\tag{ev-MIQP}
$$

Notes on the two relaxations

The steps are almost the same.

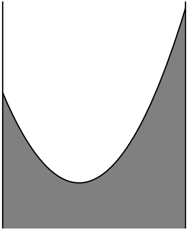
- If Q is diagonal the two relaxations are identical.
- In general they are not comparable.
- If $Q \succeq 0$, EV-space is better it preserves convexity.
- Q-space gives a surpisingly good approximation [Luedtke et al., 2012] show that, if Q has a 0 diagonal, for the box QP: $\min\{x^T Qx : 0 \leq x \leq 1\}$:
  - if $Q \geq 0$ the approximation is within a factor 2:
  - if $Q \ngeq 0$ the approximation is within a factor of $\#$ nnz in Q (conjecture it is better)
  - Many ways to do different splittings of Q for eg. with SDP [Billionnet et al., 2012].

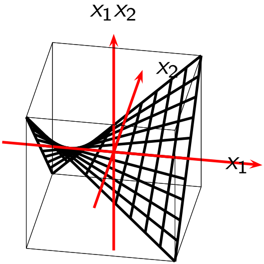
CPLEX strategy

- By default, uses EV-space if problem looks almost convex.
- Can be controled with parameter.

Branching

- Let $(\overline{x}, \overline{y})$ be the solution of the chosen QP relaxation after presolve/cutting. And assume $x_j \in \mathbb{Z}$, $j = 1, \ldots, p$.
- If $\exists \overline{y}_{ij} \neq \overline{x}_i \overline{x}_j$, $(\overline{x}, \overline{y})$ is not a solution of the problem and we need to branch.
- Pick such an index i, choose a value θ between $\frac{l_i + u_i}{2}$ and $\overline{x}_i$.
- Branch by changing the bound to θ and updating all Secant and McCormick approximations involving this bound.





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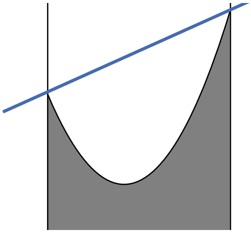

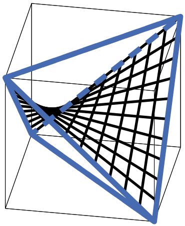

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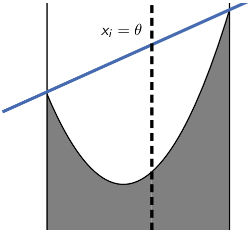

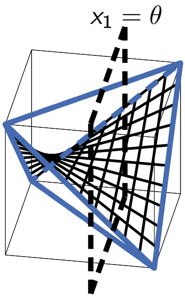

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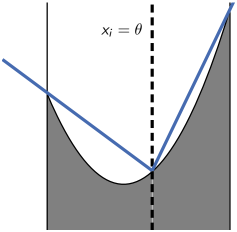

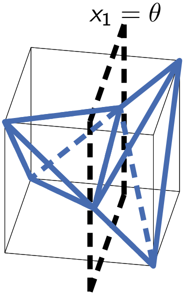

Going beyond QP

An Optimistic outlook

- GLOMIQO[Misener and Floudas, 2013] a solver for non-convex MIQCQP was released in 03/2012.
- ANTIGONE[Misener and Floudas, 2014] generalized to MINLP was released in 06/2013.
- Both solvers improved the state of the art.
- Development done by one (very good) student!
- Apparently GLOMIQO→ANTIGONE was not that hard.

The basic of a spatial branch-and-bound remains the same but of course a lot more of technicalities.

Factorable functions

$g(x)$ is factorable if it can constructed as a finite recursive composition of functions from a finite set $\{\phi_1, \ldots, \phi_k\}$ whose arguments are either variables, constants or other factorable functions.

- The usual (minimal) set of *atomic functions* is composed of: $\phi_1(x) = \ln(x)$, $\phi_2(x) = e^x$, $\phi_3(x, y) = x + y$, $\phi_4(x, y) = xy$, $\phi_5(x, \alpha) = x^\alpha$.
- For eg., $f(x) = \sqrt{x_1 x_2} + \ln(x_2)$ can be factorized into:

$$f(x) = x_3 + x_4 = \phi_3(x_3, x_4)$$
$$x_3 = \sqrt{x_5} = \phi_5(x_5, \frac{1}{2})$$
$$x_4 = \ln(x_2) = \phi_1(x_2)$$
$$x_5 = x_1 x_2 = \phi_4(x_1, x_2)$$

- Factorizations are not unique (for eg. the function $x_1^2 x_2 + \ln(x_1 x_2^2)$)

Expression trees

Expression trees are not trees but Directed Acyclic Graphs!

Basic data structure to store functions in (MI)NLP solvers. Used for:

- Constructing relaxations,
- Propagating bounds (forward/backwards),
- Computing derivatives,
- ...
- Modelling languages (GAMS, AMPL,...) have API to access Exp. Tree

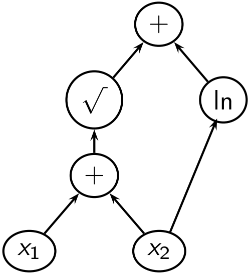

Figure: Expression tree for $f(x) = \sqrt{x_1 x_2} + \ln(x_2)$

Factorable programming relaxation

Assume all functions f and g are factorable. Adding appropriately many variables, reformulate (MINLP) as

$$\begin{array}{lll} \min & x_{n+q} & \\ \text{s.t.} & x_k = \phi_k(x) & k = n+1, n+2, \ldots, n+q \\ & x \in X & \\ & x_j \in \mathbb{Z} & j = 1, \ldots, p \\ & l_j \le x_j \le u_j & j = 1, \ldots, n+q \end{array}$$

- Now building a convex relaxation is just a matter of knowing how to relax all constraints $x_k = \phi_k(x) \Rightarrow$ Convex Envelopes.
- Build a library of convex relaxations for all atomic functions.
- Richer library $\Rightarrow$ more powerful/general solver.
  (For QP we just needed the functions $x_i x_j$ and x_i^2)

Making it work

"The factorable relaxation is the worst form of relaxation, except for all the others."

- Build rich set of atomic functions ⇒ Try to retain as much *global* information as possible.
- Recognize convex parts of problem[Vigerske, 2012].
- Elaborate tight convex envelopes [Misener and Floudas, 2014].
- Simplify expression trees.

Making it work

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- Simplify expression trees.

There are other forms of relaxation...
for eg sum-of-squares [Lasserre, 2009]

Other essential ingredients

[Tawarmalani and Sahinidis, 2002, Vigerske, 2012, Misener and Floudas, 2014]

- Use NLP solver for getting/improving incumbents.
- Linearize completely parts of the problem involving binary variables.
- Quality of any convex relaxation depends on tight bounds ⇒ aggressive propagations/bound tightening:
  - Propagate bounds forward/backward in Exp. Tree [Messine, 2004].
  - Optimality based [Gleixner and Weltge, 2013].
- Add cutting plane techniques:
  - Reformulation Linearisation Technique [Sherali and Adams, 1999].
  - Mutlilinear terms of high order [Meyer and Floudas, 2005].
  - Disjunctive [Saxena et al., 2010, Belotti, 2012].
  - SDP based.
- Branching rules [Belotti et al., 2009].
- Heuristics [Berthold and Gleixner, 2013, Berthold, 2014]

Stefan Vigerske

Part II

Selected Advanced (or not) Topics

Selected Advanced (or not) Topics

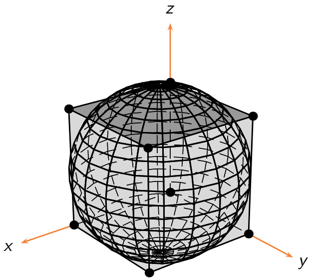
Section 3

A most simple MINLP

A simple MINLP

Consider the following convex MINLP:

$$
\begin{array}{ll}
\min & \sum_{i=1}^{n} i \times x_i \\
\text{s.t.} & \sum_{i=1}^{n} \left(x_i - \frac{1}{2}\right)^2 \le \frac{n-1}{4} \\
 & x \in \mathbb{Z}^n
\end{array}
\qquad (1)
$$



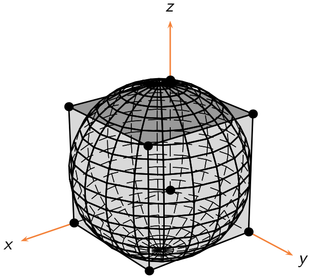
Exercise

- Find the optimum or prove that (1) is infeasible or unbounded.
- How many nodes, would a simple branch-and-bound take to solve (1)?
- How many linear approximations would an Outer Approximation approach need?
- You can use your favourite solver to help with the answers
  - ZIMPL+SCIP is fine.
  - No need to take large n (10 to 20 is fine).

Answers

Consider the following convex MINLP:

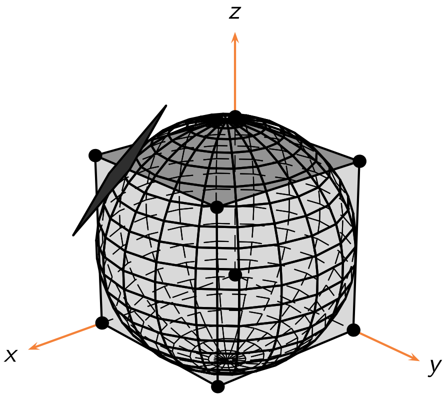
$$
\begin{array}{ll}
\min & \sum_{i=1}^{n} i \times x_i \\
\text{s.t.} & \sum_{i=1}^{n} \left(x_i - \frac{1}{2}\right)^2 \leq \frac{n-1}{4} \\
& -10 \leq x \leq 10, x \in \mathbb{Z}^n
\end{array} \qquad (1)
$$



- (1) is infeasible:
  - The ball is too small to contain integer points.
  - It is large enough to touch every edge of the hypercube.
- A basic branch-and-bound would take at least 2^{n+1} nodes.
- We need at least 2^n linear outer approximations to prove infeasibility.

Solving (1) with OA cuts

- No OA constraint can cut 2 vertices of the hypercube.
  - If an inequality cuts two points, it cuts the segment joining them.
  - The ball has a non-empty intersection with every segment joining two vertices.
  - Remember that an outer approximation is only a tangent to the ball.



What did the solvers tell?

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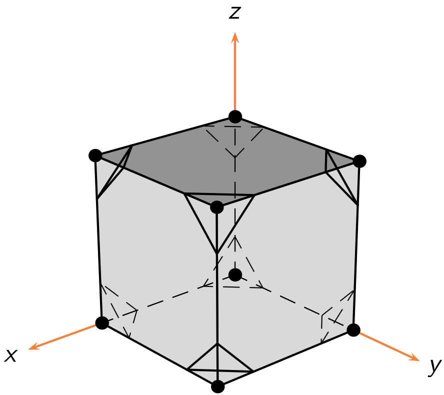

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A few years ago

		CPLEX 12.4	SCIP 2.0.1	B-OA	B-Hyb
n	2^n	nodes	nodes	OA it.	nodes

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Remark

- Problem is trivial if variables are $0-1$: replace x_i^2 by x_i, the contradiction $\frac{n}{4} \leq \frac{n-1}{4}$ follows.

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Remark

- Problem is trivial if variables are $0-1$: replace x_i^2 by x_i, the contradiction $\frac{n}{4} \leq \frac{n-1}{4}$ follows.
- SCIP $\geq$ 2.1 and CPLEX $\geq$ 12.6.1 solve it in a blink.

Solving the problem by presolve/propagation

An easy way to deduce infeasibility is to compute the component-wise maximum of the left-hand-side of the constraint:

$$\sum_{i=1}^{n} \min\left\{\left(x_i - \frac{1}{2}\right)^2 : x_i \in \mathbb{Z}\right\}$$

Each optimization problem is one dimensional and can be easily solved:

$$\min\left\{\left(x_i - \frac{1}{2}\right)^2 : x_i \in \mathbb{Z}\right\} = \frac{1}{4}$$

Summing up we get that:

$$\sum_{i=1}^{n} \min\left\{\left(x_i - \frac{1}{2}\right)^2 : x_i \in \mathbb{Z}\right\} = \frac{n}{4} > \frac{n-1}{4}.$$

A contradiction, therefore (1) is infeasible.

Twisting our example

The following model should be complicated enough to pass presolve untouched:

$$\min \sum_{i=1}^{2n} i * x_i$$
$$\sum_{i=1}^{n}(100x_{2i}^2 + 100x_{2i-1}^2 - 4x_{2i}x_{2i-1} - 98x_{2i} - 98x_{2i-1}) \leq -1 \qquad (2)$$
$$-10 \leq x \leq 10, x \in \mathbb{Z}^{2n}$$

Exercise

- Try to write a model with ZIMPL and solve it with a solver of your choice (SCIP is fine).
- How many nodes, does it take?
- No need to take large n, around 10 is fine.
- Note that the dimension of the problem is $2n$.

A recipe for solving (2) better with OA

We consider a specific class of MINLPs:

$$\begin{array}{lll} \min & c^T x & \\ \text{s.t.} & g_i(x) \leq 0 & i = 1, \ldots, m \\ & x \in X & \\ & x_j \in \mathbb{Z} & j = 1, \ldots, p \\ & l \leq x \leq u & \end{array} \qquad \text{(sMINLP)}$$

- For $i = 1, \ldots, m$, $g_i : X \to R$ are *convex separable*:

$$g_i(x) = \sum_{j=1}^{n} g_{ij}(x_j)$$

with $g_{ij} : [l_j, u_j] \to \mathbb{R}$ convex.

Disaggregated formulation

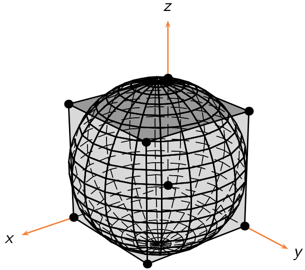
Introduce one variable y_{ij} for each elementary function:

$$
\begin{aligned}
\min \quad & c^T x \\
\text{s.t.} \quad & \sum_{j=1}^{n} y_{ij} \leq 0 && i = 1, \ldots, m, \\
& g_{ij}(x_j) \leq y_{ij} && \begin{array}{l} i = 1, \ldots, m, \\ j = 1, \ldots, n, \end{array} \\
& x \in X, \\
& x_i \in \mathbb{Z} && i = 1, \ldots, p, \\
& l \leq x \leq u.
\end{aligned}
\qquad \text{(sMINLP}^*\text{)}
$$

Application to (1)

Extended formulation of (1)

$$\begin{aligned} \min \ & c^T x \\ \text{s.t.} & \sum_{i=1}^{n} y_i \le (n-1)/4 \\ & (x_i - 0.5)^2 \le y_i \qquad i = 1, \dots, n \\ & x \in \mathbb{Z}^n. \end{aligned} \tag{3}$$



Its outer approximation

$$\begin{aligned} \min \ & c^T x \\ \text{s.t.} & \sum_{i=1}^{n} y_i \le (n-1)/4 \\ & 2\left(\overline{x}_i^k - 0.5\right)\left(x_i - \overline{x}_i^k\right) + \left(\overline{x}_i^k - 0.5\right)^2 \le y_i \qquad \begin{array}{c} i = 1, \dots, n \\ k = 1, \dots, K \end{array} \\ & x \in \mathbb{Z}^n \end{aligned}$$

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Extended formulation of (1)

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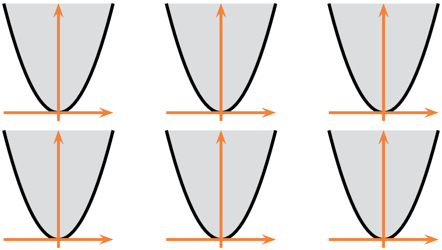

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& x \in \mathbb{Z}^n
\end{aligned}
$$

Application to (1)

Extended formulation of (1)

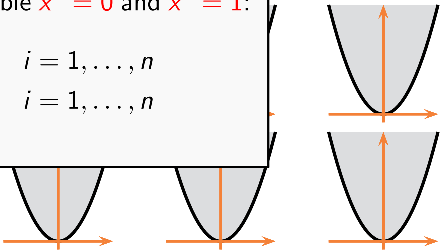
$$\min \; c^T x$$

$$\text{s.t.} \sum_{i=1}^{n} y \ldots$$

$$(x_i - \ldots$$

$$x \in \mathbb{Z}^n.$$

(3)



2 points suffice to make it infeasible $\overline{x}^1 = 0$ and $\overline{x}^2 = 1$:

$$-x_i + 0.25 \le y_i \qquad i = 1, \ldots, n$$

$$x_i - 0.75 + \le y_i \qquad i = 1, \ldots, n$$

Its outer approximation

$$\min \; c^T x$$

$$\text{s.t.} \sum_{i=1}^{n} y_i \le (n-1)/4$$

$$2\left(\overline{x}_i^k - 0.5\right)\left(x_i - \overline{x}_i^k\right) + \left(\overline{x}_i^k - 0.5\right)^2 \le y_i \qquad \begin{array}{c} i = 1, \ldots, n \\ k = 1, \ldots, K \end{array}$$

$$x \in \mathbb{Z}^n$$

Application to (2)

$$\min \sum_{i=1}^{2n} i * x_i$$
$$\sum_{i=1}^{n}(100x_{2i}^2 + 100x_{2i-1}^2 - 4x_{2i}x_{2i-1} - 98x_{2i} - 98x_{2i-1}) \leq -1$$
$$-10 \leq x \leq 10, x \in \mathbb{Z}^{2n}$$

Exercise

- Try to write a disagregated version with ZIMPL and solve it with a solver of your choice (SCIP is fine).
- How many nodes, does it take?

Application to (2): Solution

We need to get to from

$$\sum_{i=1}^{n}(100x_{2i}^2 + 100x_{2i-1}^2 - 4x_{2i}x_{2i-1} - 98x_{2i} - 98x_{2i-1}) \leq -1$$

to something of the form:

$$\sum_{i=1}^{n}(\alpha z_{2i} + \beta z_{2i-1} - 98x_{2i} - 98x_{2i-1}) \leq -1$$
$$y_i^2 \leq z_i$$
$$y_i = \gamma_i^T x.$$

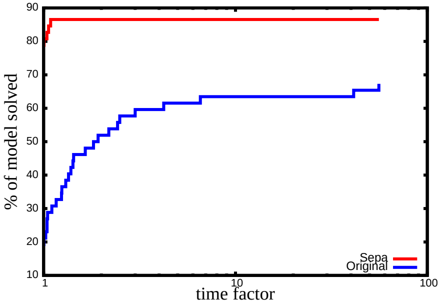
How do we find $\alpha, \beta and \gamma$?
Spectral decompostion:

$$\begin{pmatrix} 100 & -2 \\ -2 & 100 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 51 & 0 \\ 0 & 49 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$$

$$\alpha = 51, \beta = 49, \gamma_{2i} = (-1, 1), \gamma_{2i-1} = (-1, -1)$$

Experimental Illustration

- In the standard benchmark for MICP, out of > 100 instances, 8 are not directly separable.
- Constructing separated formulations on a subset of 47 instances gives a $3x$ speed up: [Hijazi et al., 14].



Similar technique developped in Baron for compositions of convex functions [Tawarmalani and Sahinidis, 2004].

Disaggregation of Second Order cones

In standard form the nonlinear constraint describing the second order cone is not convex separable:

$$\sum_{i=1}^{n} x_i^2 \le x_0^2$$

Trick [Vielma et al., 2015], divide the constraint by $x_0 \ge 0$ to get a convex separable constraint:

$$\sum_{i=1}^{n} \frac{x_i^2}{x_0} \le x_0.$$

Now introduce $y_1, \dots, y_n$ and rewrite as:

$$\sum_{i=1}^{n} y_i \le x_0$$

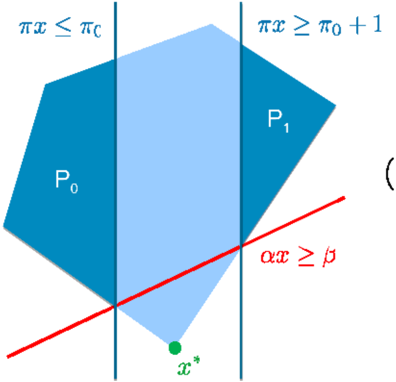
$$x_i^2 \le x_0 y_i$$

LIFT & PROJECT CUTS

CGLP magic

CGLP basics

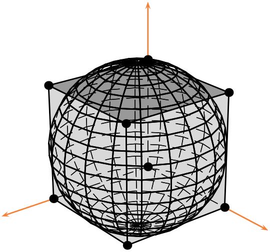
$$(u) Ax = b$$
$$(u_0) -\pi x \geq -\pi_0$$
$$x \geq 0$$



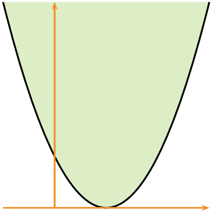
$$(v) Ax = b$$
$$(v_0) \pi x \geq \pi_0 + 1$$
$$x \geq 0$$

Going further with cutting plane

[Cornuéjols and Li, 2001] showed that the empty ball in dimension n has *split rank n*
⇒ Practically unsolvable using any known cutting plane technique.

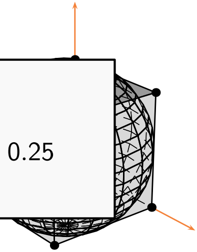


Instead the of the disaggregated formulation has (simple) split rank 1.



Going further with cutting plane

[Cornuéjol ... the empty ... *rank n* ... ⇒ Practic ... known cut



$$\left.\begin{array}{ll} -x_i + 0.25 \le y_i & i = 1, \ldots, n \\ x_i - 0.75+ \le y_i & i = 1, \ldots, n \\ x_i \le 0 \text{ OR } x_i \ge 1 & \end{array}\right\} \Rightarrow y_i \ge 0.25$$

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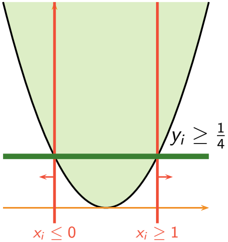
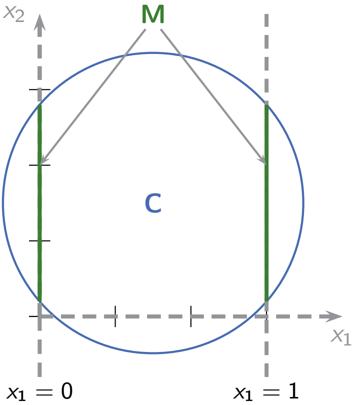


Split Relaxation

Consider $\mathbf{C}$ and $\mathbf{M} := \mathbf{C} \cap (\mathbb{Z}^p \times \mathbb{R}^{n-p})$.
Let $\pi \in \mathbb{Z}^p \times \{0\}^{n-p}$, $\pi_0 \in \mathbb{Z}$ and

$$\mathbf{C}^{(\pi,\pi_0)} := \mathrm{conv}\Big(\mathbf{C} \cap \big(\{x : \pi^T x \le \pi_0\} \cup \{x : \pi^T x \ge \pi_0 + 1\}\big)\Big).$$

(clearly $\mathbf{M} \subseteq \mathbf{C}^{(\pi,\pi_0)} \subseteq \mathbf{C}$).



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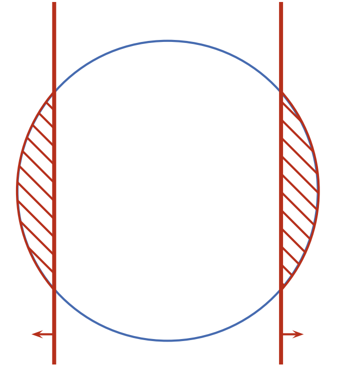

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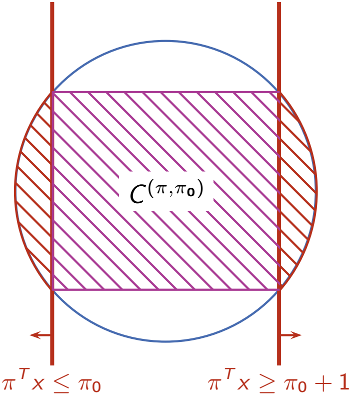

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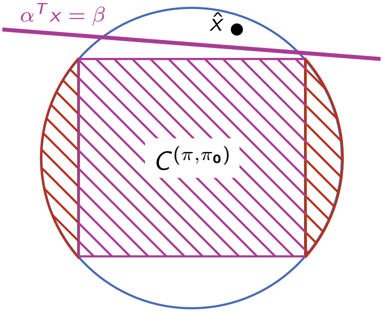
(clearly $\mathbf{M} \subseteq \mathbf{C}^{(\pi,\pi_0)} \subseteq \mathbf{C}$).

In the remainder, $\hat{x}$ is the point to separate,
$\pi = e_k$, $\hat{x}_k \in]0,1[$ $(k \leq p)$, and $\pi_0 = 0$



MILP case

Consider a polyhedron $P := \{x : Ax = b, x \geq 0\}$

Cut Generation LP [Balas, 1979, Balas et al., 1993]

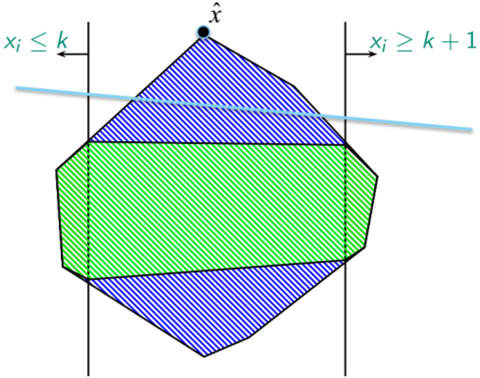
$\hat{x} \in P$ is separated from $P^{(e_k,0)}$ using the LP:

$$
\begin{aligned}
&\min \alpha^T \hat{x} - \beta \\
&s.t.: \\
&\alpha = u^T A - u_0 e_k, \qquad \alpha = v^T A + v_0 e_k, \\
&\beta = u^T b, \qquad \beta = v^T b + v_0, \\
&\alpha \in \mathbb{R}^n, \beta \in \mathbb{R}, u, v \in \mathbb{R}^m, u_0, v_0 \in \mathbb{R}_+
\end{aligned}
\tag{CGLP}
$$

If $\hat{x} \notin P^{(e_k,0)}$, $\alpha^T x \geq \beta$ cuts $\hat{x}$; otherwise produces certificate that $\hat{x} \in P^{(e_k,0)}$ with $x^0 \in P \cap \{x_k = 0\}$, $x^1 \in P \cap \{x_k = 1\}$ such that $\hat{x} = \hat{x}_k x^1 + (1 - \hat{x}_k) x^0$.

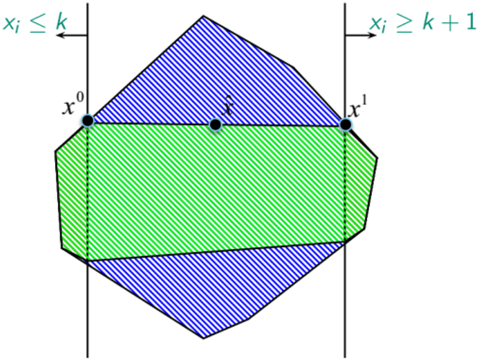
Statement in picture

If $\hat{x}$ is not in the split relaxation we get a cut.



Statement in picture

If $\hat{x}$ is in the split relaxation we get a certificate in the form of two points x^0, x^1.



MILP case (primal view)

Membership LP [Bonami, 2012]

$\hat{x} \in P$ wih $0 < \hat{x}_k < 1$ also in $P^{(e_k,0)}$ if $\exists\ x^0 \in P \cap \{x_k = 0\}$ and $x^1 \in P \cap \{x_k = 1\}$ with $\hat{x} = \hat{x}_k x^1 + (1 - \hat{x}_k)x^0$, or if

$$\begin{aligned} &\max\ y_k \\ &\text{s.t.} \\ &Ay = b\hat{x}_k \\ &0 \le y \le \hat{x}, \\ &y \in \mathbb{R}^n. \end{aligned} \tag{MLP}$$

has a solution with $y_k = \hat{x}_k$ otherwise can deduce a cut from dual optimal solution.
(Hint $\frac{y}{\hat{x}_k}$ is x^1, $\frac{\hat{x}-y}{1-\hat{x}_k}$ is x^0).

Generalization to MICPs

Using the primal view

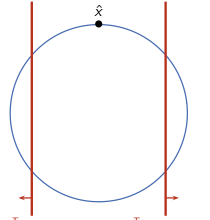
- Generalizing (MLP) to nonlinear convex constraints is relatively simple [Bonami, 2011].
- But Nonlinear programming duality is not the same as LP!

Using the dual view

- Generalizing CGLP is possible but poses many numerical/technical challenges[Ceria and Soares, 1999, Stubbs and Mehrotra, 1999].
- As long as we generate a linear cut, it can be obtained from linear outer approximations[Bonami et al., 2012].
- The linear case can be used within a cut generation framework [Kılınc et al., 2011].

Sketch of an algorithm

- Only solve LPs,
- Dynamic generation of additional OA constraints.
- compact formulation using MLP,



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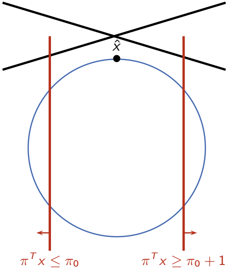

Sketch of an algorithm

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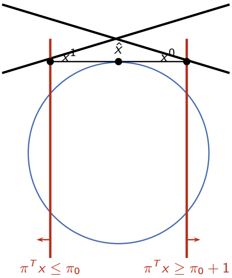
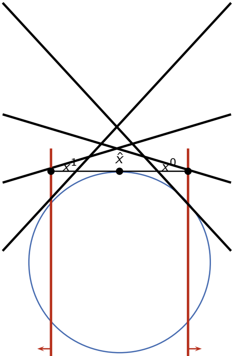


Sketch of an algorithm



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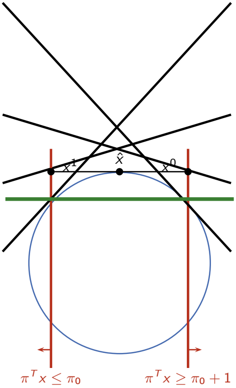
Sketch of an algorithm



- Only solve LPs,
- Dynamic generation of additional OA constraints.
- compact formulation using MLP,

In CPLEX

- Propagation of conic constraints (12.6.1).
- Cone disaggregation for MISOCP (12.6.2).
- Lift-and-project cuts for MISOCP (12.6.2).
- Redesigned heuristic choice of most promising algorithm (12.6.2).
- Improved OA Cuts (12.6.2).

The effect on our ellipse

$$\min \sum_{i=1}^{2n} i * x_i$$
$$\sum_{i=1}^{n}(100x_{2i}^2 + 100x_{2i-1}^2 - 4x_{2i}x_{2i-1} - 98x_{2i} - 98x_{2i-1}) \leq -1 \qquad (2)$$
$$x \in \mathbb{Z}^{2n}$$

- results on 12 threads with 12.6.1, 12.6.2[2], 12.6.2-- (no lift-and-project cuts) and 12.6.2++ (aggressive lift-and-project cuts), 3 hours time limit

	12.6.1	12.6.2--	12.6.2	12.6.2++
n	nodes	nodes	nodes	nodes
5	2,261	2,045	2,045	1,825
10	2,097,151	1,914,797	29	1
15	>23,125,426	>146,604,478	7,769	1

(Largest model solved in 2.2 sec by 12.6.2, in 5.5 sec by 12.6.2++.)

[2] Default results can be very sensitive to objective function

The effect on our ellipse

Similar results previously observed by [Kılınç, 2011]

		Original		Disaggregated	
	n	root gap	sol time	root gap	sol time
Batch	10	58.40	376.2	68.77	58.7
Markowitz	10	0.00	> 10 800	98.07	1 262
SLay	14	68.50	36	86.08	5.0
uflquad	15	10.85	784	96.25	145

cuts) and 12.6.2++ (aggressive lift and project cuts), 3 hours time limit

	12.6.1	12.6.2--	12.6.2	12.6.2++
n	nodes	nodes	nodes	nodes
5	2,261	2,045	2,045	1,825
10	2,097,151	1,914,797	29	1
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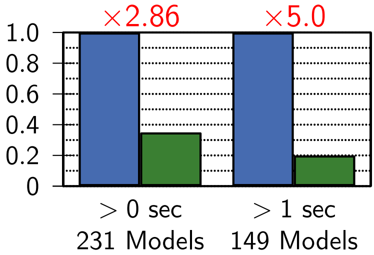
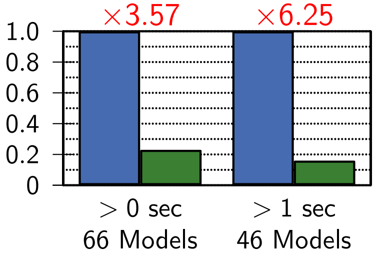
[2] Default results can be very sensitive to objective function

CPLEX 12.6.1 vs 12.6.2



CPLEX test bed

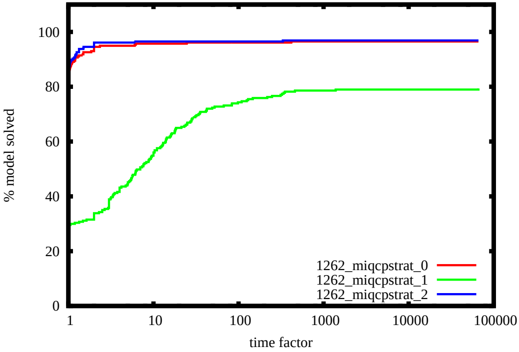
- CPLEX 12.6.1: 62 time limits
- CPLEX 12.6.2: 38 time limits



CBLIB

- CPLEX 12.6.1: 17 time limits
- CPLEX 12.6.2: 8 time limits

A comparison of OA and SOCP-BB in CPLEX 12.6.2 [3]



Default strategy picked

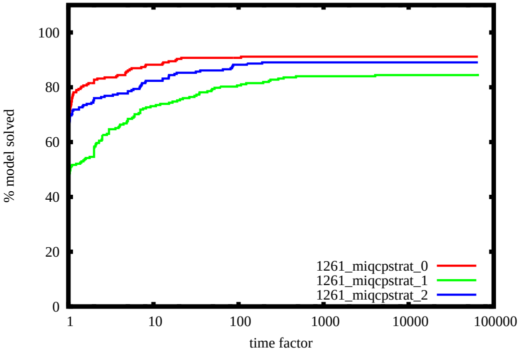
- OA 186 times
- SOCP-BB 4 times
- 55 models identical with both

To be perfect should have picked

- 2 more models with OA
- 9 more models with SOCP-BB

[3] 245 models solved by at least one method and failed by none.

Reminder of CPLEX 12.6.1 [4]



Default strategy picked

- OA 113 times
- SOCP-BB 46 times
- 56 models identical with both

To be perfect should have picked

- 14 more models with OA
- 36 more models with SOCP-BB

[4] 225 models solved by at least one method and failed by none.

Selected Advanced (or not) Topics

Section 4

MILP vs. Non-Convex QP

Box QP

We consider the box constrained QP:

$$\begin{aligned} &\max \ \frac{1}{2}x^T Qx + c^T x \\ &s.t. \\ &\qquad 0 \leq x \leq 1 \end{aligned} \qquad \text{(box-QP)}$$

- Bounds 0 and 1 are without loss of generality (every box QP can be scaled to those bounds).
- Academic interest [Vandenbussche and Nemhauser, 2005, Burer and Vandenbussche, 2009, Chen and Burer, 2012]
- Also some applications [Moré and Toraldo, 1989] (usually huge size).

The HP Property

Consider a box-QP:

$$\max \frac{1}{2}x^T Qx + c^T x \quad \text{(box-QP)}$$
$$s.t.$$
$$0 \leq x \leq 1$$

If $q_{ii} \geq 0$ then in an optimal solution $x_i \in \{0, 1\}$.

Proof

In dimension 1 ??

The HP Property

Consider a box-QP:

$$\begin{aligned} \max\ & \frac{1}{2}x^T Qx + c^T x \\ s.t.\ & \\ & 0 \leq x \leq 1 \end{aligned} \qquad \text{(box-QP)}$$

If $q_{ii} \geq 0$ then in an optimal solution $x_i \in \{0, 1\}$.

Proof

In dimension 1 $\max qx^2 + ax + c$ over $x \in [0, 1]$ and with $q \geq 0$ has its optimal solution at one end of the interval $[0, 1]$.

The HP Property

Consider a box-QP:

$$\begin{aligned} \max\ & \frac{1}{2}x^T Qx + c^T x \\ s.t.\ & \\ & 0 \leq x \leq 1 \end{aligned} \qquad \text{(box-QP)}$$

If $q_{ii} \geq 0$ then in an optimal solution $x_i \in \{0, 1\}$.

Proof

In dimension 1 $\max qx^2 + ax + c$ over $x \in [0, 1]$ and with $q \geq 0$ has its optimal solution at one end of the interval $[0, 1]$.

In dimension n. Suppose $q_{ii} \geq 0$ and $\bar{x}$ with $\bar{x}_1 \in]0, 1[$.

Consider the 1-d optimization problem where all variables are fixed to their value in $\bar{x}$ except x_1.

This problem has optimal solution in either $x_1 = 0$ or $x_1 = 1$, so we get a better solution (of course it is feasible since there are no constraints).

Why would that be useful?

Consider a box-QP with all $q_{ii} \geq 0$ then it has the same optimal solution as:

$$\max_{x \in \{0,1\}} \frac{1}{2} x^T Q x + c^T x \qquad \text{(bin-QP)}$$

Hands on with ZIMPL

Try to build a random box-QP and solve it as a continuous problem and {0-1} problem.

- You can generate a random matrix with ≥ 0 diagonal with:

```
param Q [<i,j> in N*N] := if i != j then random (-10,10)
                                    else random (-10, 0) end;
```

- ZIMPL doesn't support quadratic objective (☹?!) you need to put it as a constraint.
- No need to make it large $n = 30$ more than fine.
- Can solve with SCIP.
- Be careful with computers ☺

Solving bin-QP

Assume that Q is without diagonal term ($Q_{ii} = 0$, $i = 1, \dots, n$), and consider the set

$$\text{conv}\left((x, Y) \in Y^Q : x \in [0,1]^n\right) = \text{conv}\left((x, Y) \in Y^Q : x \in \{0,1\}^n\right).$$

- This set is called Boolean Quadratic Polytope (BQP) [Padberg, 1989].
- It is also equivalent to the Max-Cut polytope [Barahona and Mahjoub, 1986].
- An important class of facets are triangle inequalities and odd-hole inequalities.
- Those inequalities are all the Chátal-Gomory cuts for the continuous relaxation[O. Günlük et al., 2015].
- They are also $0 - 1/2$ CG cuts for which modern solvers have good heuristic separators.

bin-QP as a relaxation of box-QP

Given a box-QP (with possibly ≥ 0 diagonal coefficients) construct a bin-QP with same Q but except 0 on the diagonal.

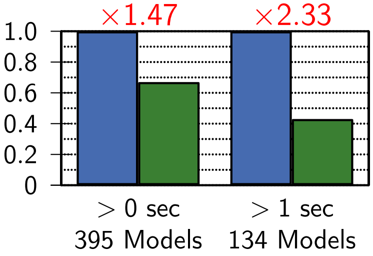
- Gives a relaxation of box-QP.
- Valid cuts for one are valid for the other.
- In particular we are interested in the $0 - 1/2$ CG cuts.
- Any non-convex QP works after removing all constraints but bounds.

Related Global Optimization approaches

Studying directly the feasible set of (box-QP) with 0 diagonal

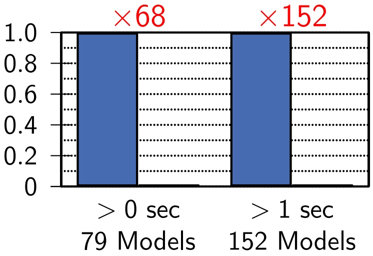
- The McCormick formula give the convex hull of 2-d box-QP sets.
- [Meyer and Floudas, 2005] give closed form formula for 3-d box-QP sets.
- Exploit closed form formula for set with up to 6 variables [Misener and Floudas, 2013].

Nonconvex (MI)QP CPLEX 12.6.1 vs 12.6.2



CPLEX test bed

- CPLEX 12.6.1: 270 time limits
- CPLEX 12.6.2: 262 time limits



Box QP

- CPLEX 12.6.1: 55 time limits
- CPLEX 12.6.2: 19 time limits

Selected Advanced (or not) Topics

Section 5

Everything can go wrong...

No need to be big to go wrong

Consider the following non-convex QP:

$$\begin{aligned} &\min \; x^2 - y^2 \\ &s.t. \\ &-1 \leq x - y \leq 1 \\ &x, y \in \mathbb{R} \end{aligned}$$

Questions

- Find the optimal solution, or prove that the problem is either infeasible or unbounded.
- Encouragements to try with a solver to see what happens (even if the answer looks obvious).

Answer

The problem is a relaxation of: $\min\{x^2 - y^2 : x - y = 1, x, y \in \mathbb{R}\}$. We show that his problem is unbounded the result follows.

Basic algebra $x^2 - y^2 = (x - y)(x + y)$ with $x - y = 1$ changes objective to $x + y$.

Now eliminate y using $y = x - 1$ and obtain $\min\{2x - 1 : x \in \mathbb{R}\}$ which is unbounded.

What happened in the solver?

In an MILP with *rational data*

If the continuous relaxation is unbounded then

- If there is an integer feasible solution $\Rightarrow$ unbounded.
- If there is no integer feasible solution $\Rightarrow$ infeasible.

In an MINLP

- It can happen that relaxation is unbounded but problem is bounded.
- Note that here we don't have integer variables but still deciding if a QP is unbounded is NP-hard.
- [Hu et al., 2012] propose an algorithm to detect correcty unbounded QPs.
- Most solvers, will continue optimization even with an unbounded relaxation.
- CPLEX tries to detect unbounded models. If relaxation is unbounded but can't decide that problem is also, stops with `RELAXATION_UNBOUNDED`.

Conclusion

- MINLP is still very challenging.
- Some significant applications solved but many still out of reach.
- According to Stefan the MINLP accelerates at a rate of $1.96/\mathit{year}$ (more than MILP's 1.8!).
- Conjecture: 25 years from now MINLPs will be solved 2.024×10^7 faster than today.
- To get there we need:

- more applications:
  `www.minlp.org`,
- more benchmark instances:
  `www.gamsworld.org/minlp/minlplib2/html/`
- more clever people:

Conclusion

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- more clever people:

IBM®

Legal Disclaimer

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