Mixed-Integer Nonlinear Optimization: Applications, Algorithms, and Computation III

Sven Leyffer

Mathematics & Computer Science Division
Argonne National Laboratory

Graduate School in
Systems, Optimization, Control and Networks
Université catholique de Louvain
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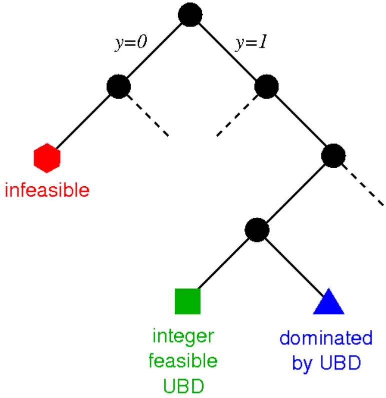
Outline

Recall: Nonlinear Branch-and-Bound

$$\underset{x}{\text{minimize}} \ f(x) \quad \text{subject to } c(x) \le 0,\ x \in X,\ x_i \in \mathbb{Z}\ \forall\ i \in I$$

Solve continuous relaxation (NLP) ($0 \le x_I \le 1$)
...solution value provides lower bound

- Branch on x_i non-integral
- Solve NLPs & branch until
  1. Node infeasible: ●
  2. Node integer feasible: □
     $\Rightarrow$ get upper bound (U)
  3. Lower bound $\ge U$: ▲

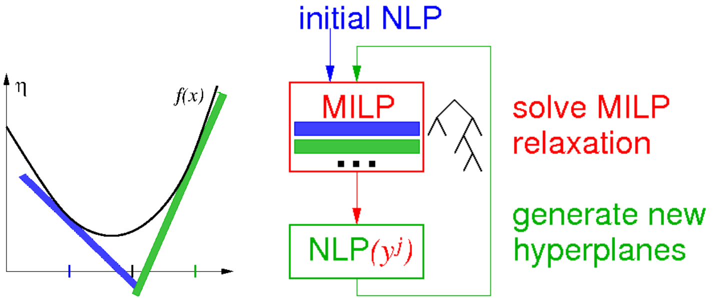


Search until no unexplored nodes

Snag: Solve thousands of NLPs ...

Recall: Outer Approximation

Alternate between solve NLP(x_I) and MILP relaxation



MILP $\Rightarrow$ lower bound; NLP $\Rightarrow$ upper bound

Snag: Solve multiple MILPs ...

Outline

Single-Tree Methods

Goal: perform only a single MILP tree-search per MINLP

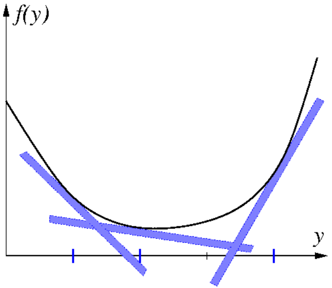
- Branch-and-Bound is s single-tree method
  ... but can be too expensive per node
- Avoid re-solving MILP master for OA, Benders, and ECP
  ... instead update master (MILP) data
- Can be interpreted as branch-and-cut approach
  ... but cuts are very simple
- Solve MILP with full set of linearizations $\mathcal{X}$ and apply delayed constraint generation technique of "formulation constraints" $\mathcal{X}^k \subset \mathcal{X}$.
- At integer points, separate cuts by solving an NLP

... basis for state-of-the-art convex MINLP solvers

LP/NLP-Based Branch-and-Bound

Aim: avoid solving expensive MILPs

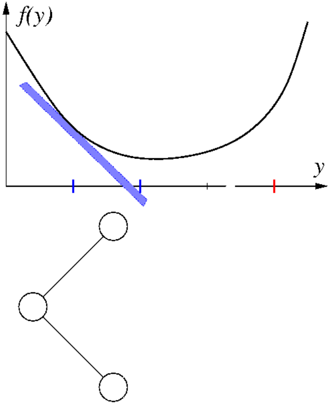
- Form MILP outer approximation



LP/NLP-Based Branch-and-Bound

Aim: avoid solving expensive MILPs

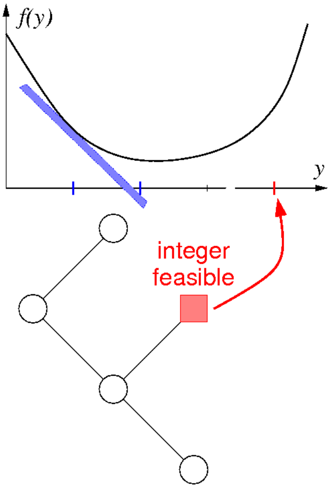
- Form MILP outer approximation
- Take initial MILP tree



LP/NLP-Based Branch-and-Bound

Aim: avoid solving expensive MILPs

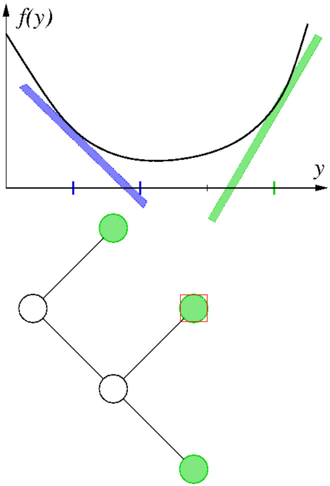
- Form MILP outer approximation
- Take initial MILP tree
- interrupt MILP, when new integral $x_I^{(j)}$ found
  $\Rightarrow$ solve NLP($x_I^{(j)}$) get $x^{(j)}$



LP/NLP-Based Branch-and-Bound

Aim: avoid solving expensive MILPs

- Form MILP outer approximation
- Take initial MILP tree
- interrupt MILP, when new integral $x_I^{(j)}$ found
  $\Rightarrow$ solve NLP($x_I^{(j)}$) get $x^{(j)}$
- linearize f, c about $x^{(j)}$
  $\Rightarrow$ add linearization to tree

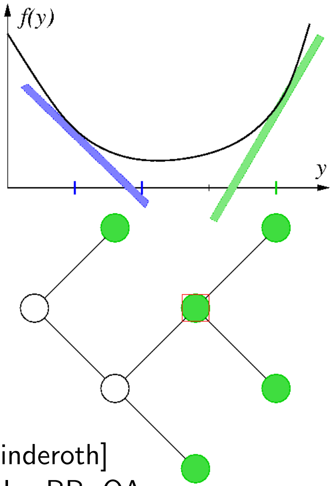


LP/NLP-Based Branch-and-Bound

Aim: avoid solving expensive MILPs

- Form MILP outer approximation
- Take initial MILP tree
- interrupt MILP, when new integral $x_I^{(j)}$ found
  $\Rightarrow$ solve NLP($x_I^{(j)}$) get $x^{(j)}$
- linearize f, c about $x^{(j)}$
  $\Rightarrow$ add linearization to tree
- continue MILP tree-search

... until lower bound $\geq$ upper bound



Software:
`FilMINT`: FilterSQP + MINTO [L & Linderoth]
`BONMIN`: IPOPT + CBC [IBM/CMU] also BB, OA

Branch-and-Cut in MINOTAUR

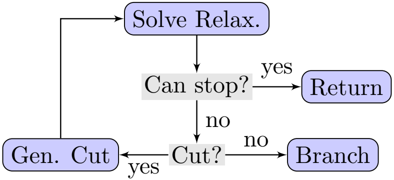
Suppose we need a branch-and-cut solver.

Node Relaxer

Obtain linear relaxation in root node.

Only CxLinHandler

Node Processor



CxLinHandler
IntVarHandler

Brancher

Pick a fractional variable.

Only IntVarHandler

```
relax() {
// Solve NLP
// get Linearization at sol.
}
bool isFeasible() {
// check non-linear constraints
}
```

```
separate() {
// solve NLP
// get Linearization at sol.
}
cand* findBrCandidates() {
// empty
}
```

LP/NLP-Based Branch-and-Bound

Algorithmic refinements, e.g. [Abhishek et al., 2010]

- Advanced MILP search and cut management techniques
  ... remove "old" OA cuts from LP relaxation ⇒ faster LP
- Generate cuts at non-integer points: ECP cuts are cheap
  ... generate cuts early (near root) of tree
- Strong branching, adaptive node selection & cut management
  - Fewer nodes, if we add more cuts (e.g. ECP cuts)
  - More cuts make LP harder to solve
    ⇒ remove outdated/inactive cuts from LP relaxation

  ... balance OA accuracy with LP solvability
- Compress OA cuts into Benders cuts can be OK

Interpret as hybrid algorithm, [Bonami et al., 2008]

Benders and ECP versions are also possible.

Outline

Presolve for MINLP

Presolve plays key role in MILP solvers

- Bound tightening techniques
- Checking for duplicate rows
- Fixing or removing variables
- Identifying redundant constraints

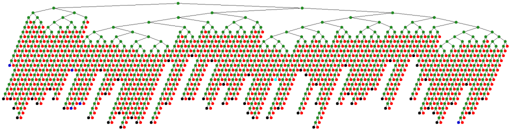
... creates tighter LP/NLP relaxations $\Rightarrow$ smaller trees!

... some presolve in AMPL, but no nonlinear presolve

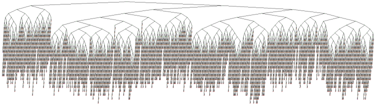
What Could Go Wrong in MINLP?

Syn20M04M : a synthesis design problem in chemical engineering

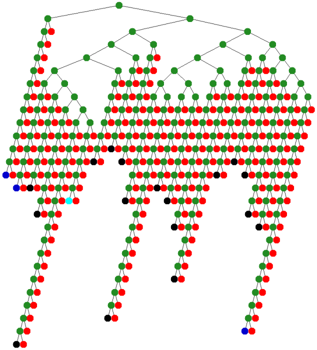
Problem size: 160 Integer Variables, 56 Nonlinear constraints



1000+ nodes after solving for 75s



5000+ nodes after solving for 200s



250+ nodes after solving for 45s

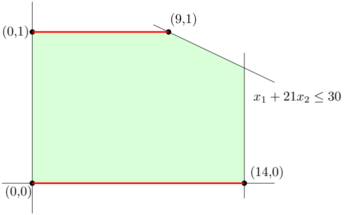
Solver	CPU	Nodes
Bonmin	>2h	>149k
MINLPBB	>2h	>150k
Minotaur	>2h	>264k

Improving Coefficients: An Example

$$
\begin{aligned}
(1) \quad x_1 + 21x_2 &\leq 30 \\
0 \leq x_1 &\leq 14 \\
x_2 &\in \{0, 1\}
\end{aligned}
$$

Improving Coefficients: An Example

$$(1) \quad x_1 + 21x_2 \le 30$$
$$0 \le x_1 \le 14$$
$$x_2 \in \{0, 1\}$$



If $x_2 = 0$	If $x_2 = 1$
$x_1 + 0 \le 30$	$x_1 \le 9$
(1) is loose.	(1) is tight.

Improving Coefficients: An Example

(1) $x_1 + 21x_2 \leq 30$

$0 \leq x_1 \leq 14$

$x_2 \in \{0, 1\}$

If $x_2 = 0$

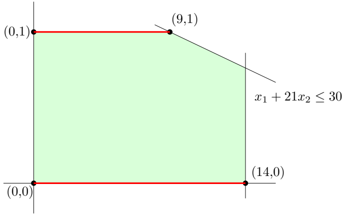
$x_1 + 0 \leq 30$

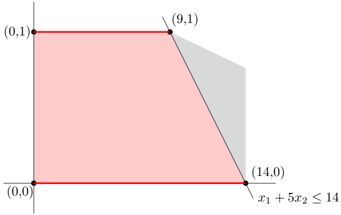
(1) is loose.

If $x_2 = 1$

$x_1 \leq 9$

(1) is tight.





Improving Coefficients: An Example

(1) $x_1 + 21x_2 \leq 30$

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$x_1 + 0 \leq 30$

(1) is loose.

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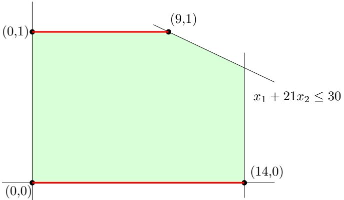
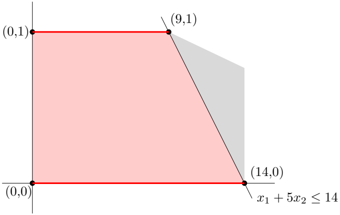
$x_1 \leq 9$

(1) is tight.





Reformulation:

(2) $x_1 + 5x_2 \leq 14$

$0 \leq x_1 \leq 14$

$x_2 \in \{0, 1\}$

If $x_2 = 0$

$x_1 + 0 \leq 14$

(2) is tight.

If $x_2 = 1$

$x_1 \leq 9$

(2) is tight.

(1) and (2) equivalent. But relaxation of (2) is tighter.

Improving Coefficients: Linear to Nonlinear

$$
\begin{aligned}
c(x_1, x_2, \ldots, x_k) &\leq M(1 - x_0) \\
l_i \leq x_i &\leq u_i, \quad i = 1, \ldots, k \\
x_0 &\in \{0, 1\}
\end{aligned}
$$

Improving Coefficients: Linear to Nonlinear

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$$

- If $c(x_1, x_2, \ldots, x_k) \le M(1 - 0)$, is loose, tighten it!

$$
\begin{aligned}
\text{Let } c^u = \max_x \; & c(x_1, \ldots, x_k) \qquad \text{(MAX-c)} \\
\text{s.t.} \; & l_i \le x_i \le u_i, \quad i = 1, \ldots, k
\end{aligned}
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- If $c^u < M$, then tighten: $c(x_1, \ldots, x_k) \le c^u(1 - x_0)$

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\end{aligned}
$$

- If $c^u < M$, then tighten: $c(x_1, \ldots, x_k) \leq c^u(1 - x_0)$
- (MAX-c) is a nonconvex NLP ... time-consuming
- Upper bound on (MAX-c) will also tighten
- Trade-off between time and quality of bound: Fast or Tight!

Improving Coefficients: Using Implications

$$
\begin{aligned}
c(x_1, x_2, \ldots, x_k) &\le M(1 - x_0), \\
l_i \le x_i &\le u_i, \quad i = 1, \ldots, k, \\
x_0 &\in \{0, 1\}.
\end{aligned}
$$

- Often, x_0, x_i also occur in other constraints of MINLP. e.g.

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\begin{aligned}
c(x_1, x_2, \ldots, x_k) &\le M(1 - x_0) \\
0 \le x_1 &\le M_1 x_0 \\
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&\ldots \\
x_0 &\in \{0, 1\}
\end{aligned}
$$

- $x_0 = 0 \Rightarrow x_1 = x_2, \ldots = x_k = 0$. (Implications)
- If $c(0, \ldots, 0) < M$, then we can tighten.

Improving Coefficients: Using Implications

$$\begin{aligned} c(x_1, x_2, \ldots, x_k) &\le M(1 - x_0), \\ l_i \le x_i &\le u_i, \quad i = 1, \ldots, k, \\ x_0 &\in \{0, 1\}. \end{aligned}$$

- Often, x_0, x_i also occur in other constraints of MINLP. e.g.

$$\begin{aligned} c(x_1, x_2, \ldots, x_k) &\le M(1 - x_0) \\ 0 \le x_1 &\le M_1 x_0 \\ 0 \le x_2 &\le M_2 x_0 \\ &\ldots \\ x_0 &\in \{0, 1\} \end{aligned}$$

- $x_0 = 0 \Rightarrow x_1 = x_2, \ldots = x_k = 0$. (Implications)
- If $c(0, \ldots, 0) < M$, then we can tighten.
- No need to solve (MAX-c). Fast and Tight.

Presolve for MINLP

Advanced functions of presolve (Reformulating):

- Improve coefficients.
- Disaggregate constraints.
- Derive implications and conflicts.

Basic functions of presolve (Housekeeping):

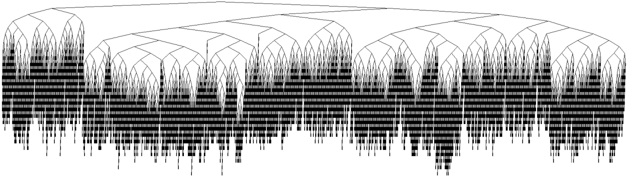
- Tighten bounds on variables and constraints.
- Fix/remove variables.
- Identify and remove redundant constraints.
- Check duplicacy.

Popular in Mixed-Integer Linear Optimization [Savelsbergh, 1994]

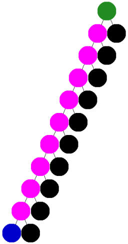
Presolve for MINLP: Computational Results

Syn20M04M from egon.cheme.cmu.edu

	No Presolve	Basic Presolve	Full Presolve
Variables:	420	328	292
Binary Vars:	160	144	144
Constraints:	1052	718	610
Nonlin. Constr:	56	56	56
Bonmin(sec):	>7200	NA	NA
Minotaur(sec):	>7200	>7200	2.3



Minotaur, no presolve: 10000+ nodes after solving for 360s

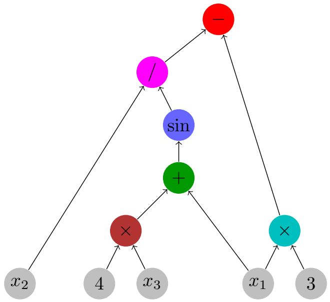


Full Presolve

Why does no one else do this?

Why Does No One else Do It? . . . Better AD!

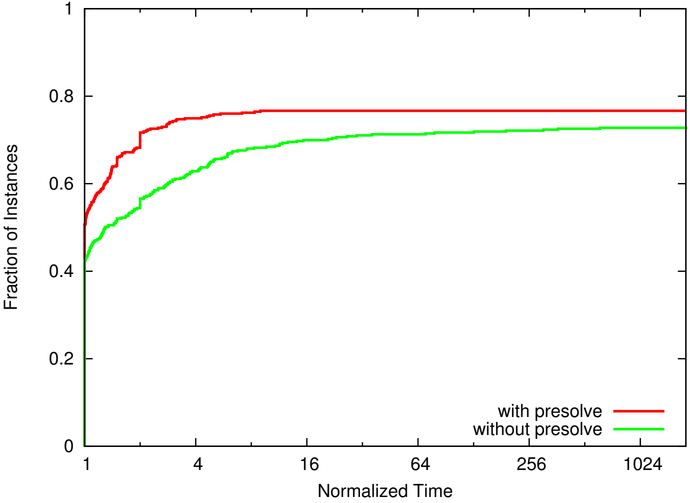
- NLP solvers need 1^{st} and 2^{nd} derivatives
- Rely on modeling software: AMPL, GAMS
  $\Rightarrow$ cannot modify functions during solve
- Minotaur has routines to
  - create computational graphs,
  - evaluate 1^{st} and 2^{nd} derivatives,
  - tighten and propagate bounds,
  - modify graphs.
- Simple modification routines:
  - Fix and delete variables.
  - Substitute variables.
  - Extract subgraphs.



$$f = \frac{x_2}{\sin(4 \times x_3 + x_1)} - 3 \times x_1$$

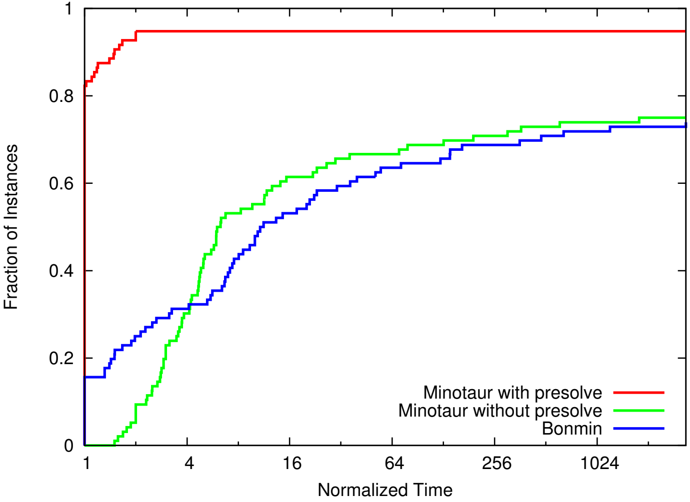
Scope for more improvements

Presolve for MINLP: Results



Time taken in Branch-and-Bound on all 463 instances.

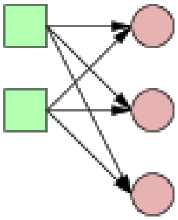
Presolve for MINLP: Results



Time for B&B on 96 RSyn-X and Syn-X instances.

Presolve for MINLP: Constraint Disaggregation

[Wolsey, 1998] uncapacitated facility location



- Set of customers $i = 1, \dots, m$
- Set of facilities $j = 1, \dots, n$
- Which facilities should we open ($x_j \in \{0, 1\}, \; j = 1, \dots, n$)
- $y_{ij} = 1$ if facility j serves customer i

Every customer served by one facility:

$$\sum_{j=1}^{n} y_{ij} = 1, \; \forall i = 1, \dots, m, \quad \text{and} \quad \sum_{i=1}^{m} y_{ij} \leq m x_j, \; \forall j = 1, \dots, n,$$

Equivalent tighter formulation is (disagregated constraints):

$$\sum_{j=1}^{n} y_{ij} = 1, \; \forall i = 1, \dots, m, \quad \text{and} \quad y_{ij} \leq x_j, \; \forall i = 1, \dots, m, \; j = 1, \dots, n.$$

... modern MIP solvers detect this automatically

Presolve for MINLP: Constraint Disaggregation

Nonlinear disaggregation [Tawarmalani and Sahinidis, 2005]

$$S := \{x \in \mathbb{R}^n : c(x) = h(g(x)) \leq 0\},$$

$g : \mathbb{R}^n \to \mathbb{R}^p$ smooth convex;
$h : \mathbb{R}^p \to \mathbb{R}$ smooth, convex, and nondecreasing
$\Rightarrow c(x)$ smooth convex

Like group partial separability [Griewank and Toint, 1984]

Disaggregated formulation: introduce $y = g(x) \in \mathbb{R}^p$

$$S_d := \left\{(x, y) \in \mathbb{R}^n \times \mathbb{R}^p : h(y) \leq 0, \; y \geq g(x)\right\}.$$

Lemma

S is projection of S_d onto x.

Presolve for MINLP: Constraint Disaggregation

Consider

$$S := \{x \in \mathbb{R}^n : c(x) = h(g(x)) \le 0\},$$

and

$$S_d := \left\{(x, y) \in \mathbb{R}^n \times \mathbb{R}^p : h(y) \le 0,\ y \ge g(x)\right\}.$$

Theorem

Any outer approximation of S_d is stronger than OA of S

Given $\mathcal{X}^k := \left\{x^{(1)}, \ldots, x^{(k)}\right\}$ construct OA for S, S_d:

$$S^{oa} := \left\{x : c^{(l)} + \nabla c^{(l)^T}(x - x^{(l)}) \le 0,\ \forall x^{(l)} \in \mathcal{X}^k\right\}$$

$$S_d^{oa} := \left\{(x, y) : h^{(l)} + \nabla h^{(l)^T}(y - g(x^{(l)})) \le 0,\right.$$

$$\left. y \ge g^{(l)} + \nabla g^{(l)^T}(x - x^{(l)}),\ \forall x^{(l)} \in \mathcal{X}^k\right\},$$

[Tawarmalani and Sahinidis, 2005] show S_d^{oa} stronger than S^{oa}

Presolve for MINLP: Constraint Disaggregation

[Hijazi et al., 2010] study

$$\left\{ x : c(x) := \sum_{j=1}^{q} h_j(a_j^T x + b_j) \leq 0 \right\}$$

where $h_j : \mathbb{R} \to \mathbb{R}$ are smooth and convex

Disaggregated formulation: introduce $y \in \mathbb{R}^q$

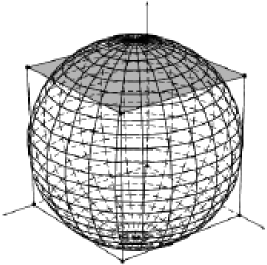
$$\left\{ (x, y) : \sum_{j=1}^{q} y_j \leq 0, \quad \text{and} \quad y_j \geq h_j(a_j^T x + b_j) \right\}$$

can be shown to be tighter

Recall: Worst Case Example of OA

Apply disaggregation to [Hijazi et al., 2010] example:

$$\begin{aligned} \underset{y}{\text{minimize}} \quad & 0 \\ \text{subject to} \quad & \sum_{i=1}^{n} \left(x_i - \frac{1}{2}\right)^2 \leq \frac{n-1}{4} \\ & x \in \{0,1\}^n \end{aligned}$$



Intersection of ball of radius $\frac{\sqrt{n-1}}{2}$ with unit hypercube.

Disaggregate $\sum \left(x_i - \frac{1}{2}\right)^2 \leq \frac{n-1}{4}$ as

$$\sum_{i=1}^{n} y_i \leq 0 \quad \text{and} \quad \left(x_i - \frac{1}{2}\right)^2 \leq y_i$$

Presolve for MINLP: Constraint Disaggregation

[Hijazi et al., 2010] disaggregation on worst-case example of OA

- Linearize around $x^{(1)} \in \{0,1\}^n$ and complement $x^{(2)} := e - x^{(1)}$, where $e = (1, \ldots, 1)$
- OA of disaggregated constraint is

$$\sum_{i=1}^{n} y_i, \quad \text{and} \quad x_i - \tfrac{3}{4} \leq y_i, \quad \text{and} \quad \tfrac{1}{4} - x_i \leq y_i,$$

- Using $x_i \in \{0,1\}$ implies $z_i \geq 0$, implies $\sum z_i \geq \frac{n}{4} > \frac{n-1}{4}$

$\Rightarrow$ OA-MILP master of $x^{(1)}$ and $x^{(2)}$ is infeasible.

... terminate in two iterations

Outline

Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & c(x) \leq 0 \\ & x \in X \\ & x_i \in \mathbb{Z} \text{ for all } i \in I \end{aligned}$$

Assumptions:

- A1 X is a bounded polyhedral set.
- A2 f and c are twice continuously differentiable convex functions.
- A3 MINLP satisfies a constraint qualification.

Look at another class of branch-and-cut methods ...

Overview of Branch-and-Cut Methods

Extend nonlinear branch-and-bound

1. Solve NLP(l, u) at each node of tree
    - Generate a cut to eliminate fractional solution & re-solve
    - Only branch if solution fractional after some rounds of cuts
2. Generation of good cuts is key [Stubbs and Mehrotra, 1999]
3. Hope that tree is smaller than BnB
4. Goal: get formulation closer to convex hull

Recall Nonlinear Branch-and-Bound

Solve NLP relaxation

$$\underset{x}{\text{minimize}} \; f(x) \quad \text{subject to } c(x) \le 0, \; x \in X$$

- If $x_i \in \mathbb{Z} \; \forall \; i \in I$, then solved MINLP
- If relaxation is infeasible, then MINLP infeasible

... otherwise search tree whose nodes are NLPs:

$$\left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & f(x), \\ \text{subject to} & c(x) \le 0, \\ & x \in X, \\ & l_i \le x_i \le u_i, \; \forall i \in I. \end{array} \right. \qquad (\text{NLP}(l, u))$$

NLP relaxation is $\text{NLP}(-\infty, \infty)$

Recall Nonlinear Branch-and-Bound

Branch-and-bound for MINLP

Choose tol $\epsilon > 0$, set $U = \infty$, add (NLP$(-\infty, \infty)$) to heap $\mathcal{H}$.

while $\mathcal{H} \neq \emptyset$ **do**

  Remove (NLP(l, u)) from heap: $\mathcal{H} = \mathcal{H} - \{$ NLP(l, u) $\}$.

  Solve (NLP(l, u)) $\Rightarrow$ solution $x^{(l,u)}$.

  if *(NLP(l, u)) is infeasible* **then**

    Prune node: infeasible

  else if $f(x^{(l,u)}) > U$ **then**

    Prune node; dominated by bound U

  else if $x_I^{(l,u)}$ *integral* **then**

    Update incumbent : $U = f(x^{(l,u)})$, $x^* = x^{(l,u)}$.

  else

    BranchOnVariable$(x_i^{(l,u)}, l, u, \mathcal{H})$

Generic Nonlinear Branch-and-Cut

Branch-and-cut for MINLP

Choose a tol $\epsilon > 0$, set $U = \infty$, add (NLP($-\infty, \infty$)) to heap $\mathcal{H}$.

while $\mathcal{H} \neq \emptyset$ **do**

Remove (NLP(l, u)) from heap: $\mathcal{H} = \mathcal{H} - \{$ NLP(l, u) $\}$.

repeat

Solve (NLP(l, u)) $\Rightarrow$ solution $x^{(l,u)}$.

if *(NLP(l, u)) is infeasible* **then**

Prune node: infeasible

else if $f(x^{(l,u)}) > U$ **then**

Prune node; dominated by bound U

else if $x_I^{(l,u)}$ *integral* **then**

Update incumbent: $U = f(x^{(l,u)})$, $x^* = x^{(l,u)}$ & prune.

else GenerateCuts($x^{(l,u)}, j$) ... details later

until *no new cuts generated or node pruned*

if *(NLP(l, u)) not pruned & not incumbent* **then**

BranchOnVariable($x_j^{(l,u)}, l, u, \mathcal{H}$)

Cut Generation Overview

Algorithm 1: Solve separation problem to generate subgradient cut

Subroutine: GenerateCuts $(x^{(l,u)}, j)$

// *Generate a valid inequality that cuts off* $x_j^{(l,u)} \notin \{0,1\}$

Solve separation (NLP) problem in $x^{(l,u)}$ for valid cut.

Add valid inequality to $(\text{NLP}(l,u))$.

GenerateCuts: valid inequality to eliminate fractional solution

- Given fractional solution $x^{(l,u)}$ with $x_j^{(l,u)} \notin \{0,1\}$.
- Let $\mathcal{F}(l,u)$ mixed-integer feasible set of node $\text{NLP}(l,u)$.
- Find cut $\pi^T x \leq \pi_0$ such that
  - $\pi^T x \leq \pi_0$ for all $x \in \mathcal{F}(l,u)$
  - $\pi^T x^{(l,u)} > \pi_0$, i.e. $x^{(l,u)}$ violates the cut
- Solve a separation problem (e.g. an NLP) for cut $\pi^T x \leq \pi_0$

... lifting cuts makes them valid throughout the tree.

Branch-and-Cut Challenges

Computational Considerations of Branch-and-Cut

- Cut-generation problem may be hard to solve
- Adds burden of additional NLP solves to BnB
  - Can solve LP instead of NLP, e.g. from OA
- Must add cut-management to solver
- Lifting cuts may help to make them valid in whole tree
- NLPs still don't hot-start

[Stubbs and Mehrotra, 1999] generate cuts only at root node

Outline

Mixed-Integer Rounding (MIR) for OA-MILP

Goal: Strengthen MILP relaxations of LP/NLP-based BnB
... iteratively add cuts to remove fractional LP solutions

Start by considering MIR cuts for "easy set"

$$S := \{(x_1, x_2) \in \mathbb{R} \times \mathbb{Z} \mid x_2 \le b + x_1,\ x_1 \ge 0\},$$

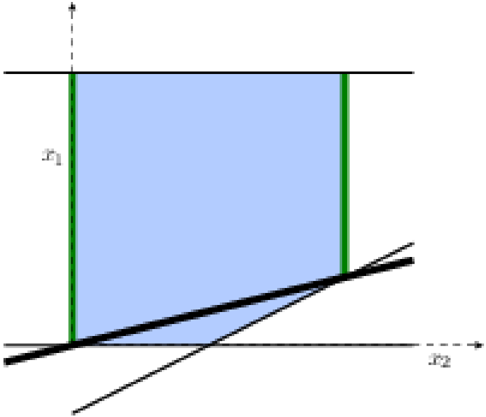
where $R = \{1\}$ and $I = \{2\}$.
Let $f_0 = b - \lfloor b \rfloor$, then cut

$$x_2 \le \lfloor b \rfloor + \frac{x_1}{1 - f_0}$$

is valid for S; look at two cases:

1. $x_2 \le \lfloor b \rfloor$
2. $x_2 \ge \lfloor b \rfloor + 1$.

Example of Simple MIR Cut



MIR cut: $x_2 \leq 2x_1$ derived from $x_2 \leq \frac{1}{2} + x_1$.

General MIR Cuts

For general MILP consider set

$$X := \{(x_R^+, x_R^-, x_I) \in \mathbb{R}_+^2 \times \mathbb{Z}_+^p \mid a_I^T x_I + x_R^+ \leq b + x_R^- \}.$$

... selected constraint row of MILP or one-row relaxation of subset

- Continuous variables aggregated in x_R^+ and x_R^- depending on sign of coefficient in a_R.
- Obtain following valid inequality:

$$\sum_{i \in I} \left(\lfloor a_i \rfloor + \frac{\max\{f_i - f_0, 0\}}{1 - f_0} \right) x_i \leq \lfloor b \rfloor + \frac{x_R^-}{1 - f_0},$$

$f_i = a_i - \lfloor a_i \rfloor$ for $i \in I$ and $f_0 = b - \lfloor b \rfloor$ fractional parts a and b.

Gomory Cuts and MIR Cuts

Gomory cuts originally from [Gomory, 1958, Gomory, 1960] for ILP
MILP Gomory cut given by

$$\sum_{i \in I_1} f_i x_i + \sum_{i \in I_2} \frac{f_0(1-f_i)}{f_i} x_i + x_R^+ + \frac{f_0}{1-f_0} x_R^- \geq f_0$$

where $I_1 = \{i \in I \mid f_i \leq f_0\}$ and $I_2 = I \setminus I_1$.
... is instance of MIR cut. Consider set

$$X = \{(x_R, x_0, x_I) \in \mathbb{R}^2_+ \times \mathbb{Z}_+ \times \mathbb{Z}^p \mid x_0 + a_I^T x_I + x_R^+ - x_R^- = b\},$$

generate a MIR inequality, and eliminate x_I^0.
In MINLP Gomory & MIR cuts generated from MILP relaxations
... [Akrotirianakis et al., 2001] report modest improvement

Outline

Perspective Formulations

MINLPs use binary indicator variables, x_b, to model nonpositivity of $x_c \in \mathbb{R}$

Model as variable upper bound

$$0 \leq x_c \leq u_c x_b, \quad x_b \in \{0,1\}$$

$\Rightarrow$ if $x_c > 0$, then $x_b = 1$

Perspective reformulation applies, if x_b also in convex $c(x) \leq 0$

- Significantly improve reformulation
- Pioneered by [Frangioni and Gentile, 2006];
  ... strengthen relaxation using perspective cuts

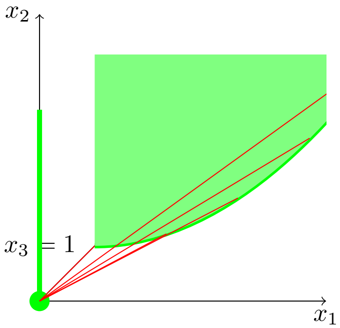
Example of Perspective Formulation

Consider MINLP set with three variables:

$$S = \left\{ (x_1, x_2, x_3) \in \mathbb{R}^2 \times \{0,1\} \ : \ x_2 \geq x_1^2, \quad u x_3 \geq x_1 \geq 0 \right\}.$$

Can show that $S = S^0 \cup S^1$, where

$$S^0 = \left\{ (0, x_2, 0) \in \mathbb{R}^3 \ : \ x_2 \geq 0 \right\},$$
$$S^1 = \left\{ (x_1, x_2, 1) \in \mathbb{R}^3 \ : \ x_2 \geq x_1^2, \ u \geq x_1 \geq 0 \right\}.$$



Example of Perspective Formulation

Geometry of convex hull of S:
Lines connecting origin ($x_3 = 0$) to parabola $x_2 = x_1^2$ at $x_3 = 1$

Define convex hull of S as conv(S)

$$:= \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_2 x_3 \geq x_1^2,\ u x_3 \geq x_1 \geq 0, 1 \geq x_3 \geq 0, x_2 \geq 0\right\}$$

where $x_2 x_3 \geq x_1^2$ is defined in terms of perspective function

$$\mathcal{P}_f(x, z) := \begin{cases} 0 & \text{if } z = 0, \\ z f(x/z) & \text{if } z > 0. \end{cases}$$

Epigraph of $\mathcal{P}_f(x, z)$: cone pointed at origin with lower shape $f(x)$

$x_b \in \{0, 1\}$ indicator forces $x_c = 0$, or $c(x_c) \leq 0$ if $x_b = 1$ write

$x_b c(x_c / x_b)$ ...is tighter convex formulation

Generalization of Perspective Cuts

[Günlük and Linderoth, 2012] consider more general problem

$$(P) \qquad \min_{(x,z,\eta)\in\mathbb{R}^n\times\{0,1\}\times\mathbb{R}} \left\{\eta \mid \eta \geq f(x) + cz, Ax \leq bz\right\}.$$

where

1. $X = \{x \mid Ax \leq b\}$ is bounded
2. $f(x)$ is convex and finite on X, and $f(0) = 0$

Theorem (Perspective Cut)

For any $\bar{x} \in X$ and subgradient $s \in \partial f(\bar{x})$, the inequality

$$\eta \geq f(\bar{x}) + c + s^T(x - \bar{x}) + (c + f(\bar{x}) - s^T\bar{x}))(z - 1)$$

is valid cut for (P)

Stronger Relaxations [Günlük and Linderoth, 2012]

- z_R: Value of NLP relaxation
- z_{GLW}: Value of NLP relaxation after GLW cuts
- z_P: Value of perspective relaxation
- z^*: Optimal solution value

Separable Quadratic Facility Location Problems

$\|M\|$	$\|N\|$	z_R	z_{GLW}	z_P	z^*
10	30	140.6	326.4	346.5	348.7
15	50	141.3	312.2	380.0	384.1
20	65	122.5	248.7	288.9	289.3
25	80	121.3	260.1	314.8	315.8
30	100	128.0	327.0	391.7	393.2

$\Rightarrow$ Tighter relaxation gives faster solves!

Nonlinear Perspective of the Perspective

Potential Pitfalls of Perspective of $h(x) \leq 0$:

- $y h(x/y) \leq 0$ ... division by zero?
- function, gradients & Hessian may not be defined at 0
- in practice get IEEE exception messages from AMPL

Example: Stochastic Service System Design

$$
\begin{array}{ll}
\underset{x,y,z}{\text{minimize}} & \frac{v}{100} + (y - \frac{1}{4})^2 + (z - \frac{1}{2})^2 \\
\text{subject to} & z - \frac{v}{1+v} \leq 0 \\
& 0 \leq z \leq y, \quad v \geq 0, \quad y \in \{0, 1\}
\end{array}
$$

Perspective of nonlinear constraint:

$$
y \left(z/y - \frac{v/y}{1 + v/y} \right) \leq 0 \quad \Leftrightarrow \quad z - \frac{v}{1 + v/y} \leq 0
$$

... not defined at $y = 0$ even after cancellation.

Nonlinear Perspective of the Perspective

Study re-formulations:

$$
\begin{aligned}
z - \tfrac{v}{1+v/y} &\leq 0 && \text{perspective} \\
zy + zv - vy &\leq 0 && \text{smooth} \\
\sqrt{4v^2 + (y+z)^2} - 2v + y - z &\leq 0 && \text{2nd-order cone}
\end{aligned}
$$

- 2nd-order cone requires SOC solver $\Rightarrow$ no general NLPs!
- IPOPT, SNOPT et al. fail for smooth formulation:
  - "Smooth formulation is nonconvex $\Rightarrow$ NLP solvers fail"
  - BONMIN fails to solve MINLPs using smooth formulation
- BB solvers fail on perspective formulation:
  ... IEEE exception $\forall$ nodes with $y = 0$

Nonlinear Perspective on the Perspective

Nonconvex formulation: $c_1(v, y, z) = zy + zv - vy \leq 0$

- Feasible set is convex $\Rightarrow$ unique minimizer
- NLP solvers converge to unique minimum ... just very slowly!
- Look at gradient:

$$\nabla c_1 = \begin{pmatrix} z - y \\ z - v \\ y + v \end{pmatrix}$$

$\Rightarrow \nabla c_1(0) = 0^T$

$\Rightarrow c_1$ violates MFCQ at 0

- Slow convergence & failure is due to failure of MFCQ

... more next!

Gradients & Constraint Qualifications (CQ)

Let $\mathcal{F} := \{c(x) \geq 0\}$ feasible set

CQs ensure that linearizations describe $\mathcal{F}$ locally!

- LPs always satisfy a CQ
- Ensure validity of first-order (gradient/KKT) conditions
- Solvers that rely on linearization techniques work well

Mangasarian-Fromowitz Constraint Qualification (MFCQ)

1. The gradients of equality constraints linearly independent
2. For all active $\mathcal{A}$ inequality constraints $\mathcal{A}(x) := \{i : c_i(x) = 0\}$:
   $\exists s : \nabla c_i^T s < 0, \; \forall i \in \mathcal{A}$ ... strictly feasible direction

MFCQ violated by $\nabla c_1 = 0$, because $0^T s < 0$ can never hold!
... causes slow convergence of *any NLP solver*

Numerical Experience with the Bad the Perspective

Bad perspective of uncapacitated facility location problem:

$$\begin{aligned} & \underset{x,y,z}{\text{minimize}} \quad z + y \\ & \text{subject to } x^2 - zy \le 0 \quad 0 \le x \le z, \; z \in \{0,1\} \end{aligned}$$

```
Major Minor TrustRad RegParam StepNorm Constrnts  Objective Optimal Phase Step
------------------------------------------------------------------------------
    0     0       10       10        0       0.5       1.01       0     2
    1     1       10       10    0.625         0      0.385       0     2  SQP
    2     1       10       10    0.188         0     0.1875       0     2  SQP
[ ... ]
   28     1       10       10 2.79e-09         0  2.794e-09       0     2  SQP
   29     1       10       10   1.4e-09         0  1.397e-09       0     2  SQP
   30     1       10       10 6.98e-10         0  6.985e-10       2     2  SQP

ASTROS Version 2.0.2 (20100913): Solution Summary
===============================================
  Major iters     =         30 ; Minor iters     =         30 ;
  KKT-residual    =     0.4286 ; Complementarity =  1.996e-10 ;
  Final step-norm =  6.985e-10 ; Final TR-radius =         10 ;
---------------------------------------------------------------
ASTROS  Version 2.0.2 (20100913): Step got too small
```

Linear rate of convergence ... similar for MINOS, FilterSQP, ...

Remedy: Limiting Gradients for the Perspective

Goal: Compute limiting gradients for perspective as $y \to 0$

Perspective of SSSD example

$$\begin{aligned} & z - \frac{v}{1+v/y} \le 0 \\ & 0 \le z \le y \\ & v \ge 0,\ y \in \{0,1\}. \end{aligned}$$

$$\nabla c_p = \begin{pmatrix} \dfrac{-1}{(1+v/y)^2} \\ \\ \dfrac{-v^2/y^2}{(1+v/y)^2} \\ \\ 1 \end{pmatrix}$$

Objective implies
$v = z/(1-z)$ active.

Observation: $y \to 0$ implies $z \to 0$, and $v = z/(1-z) \to 0$.

$$\nabla c_p(0) \in \text{conv} \left\{ \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -\frac{1}{4} \\ -\frac{1}{4} \\ 1 \end{pmatrix} \right\}$$

... similar derivation possible for gradients of SOC formulation!

Nonlinear Perspective of the Perspective

NLP solvers for perspective constraints

- Perspective violates linear independence CQ (LICQ)
  ... OK for robust NLP solvers (work with basis)
- Limiting gradients exist & satisfy MFCQ at 0
- Hessian blows up near $y = 0$: $\nabla^2 c_p = \mathcal{O}(y^{-1})$ typically
  ... OK because null-space is empty near $y = 0$ (LICQ fails)

Modify NLP solvers & make them aware of structure

1. Use limiting gradients near 0
2. Set Hessian $\nabla^2 c_p = [0]$ near 0

$\Rightarrow$ robust & fast local convergence (proof similar to MPECs?)

Exact Smoothing of the Perspective

Changing NLP solvers is hard ... modify the perspective:

$$\underset{x,y,z}{\text{minimize}} \quad z + y$$
$$\text{subject to } \frac{x^2}{z} - y \leq 0, \quad 0 \leq x \leq z, \; z \in \{0,1\}$$

For $\tau > 0$ (e.g. $\tau = 0.1$), replace perspective by:

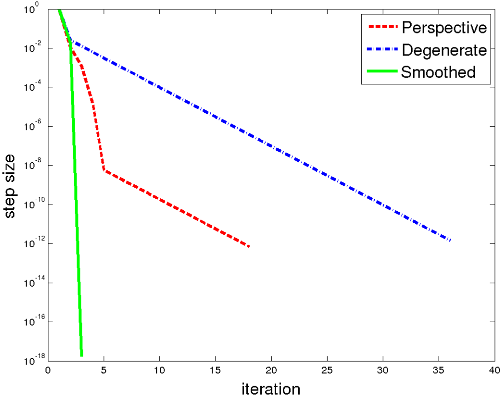
$$c_s(x,y,z) = \begin{cases} \frac{x^2}{z} - y & \text{if } z \geq \tau \\ 2x + x - y - z & \text{otherwise,} \end{cases}$$

continuously differentiable (across line $x = z = \tau$).

... readily implemented in AMPL & converges rapidly!

Nonlinear Perspective of the Perspective

Another example



... work in progress

Outline

Disjunctive Branch-and-Cut

[Stubbs and Mehrotra, 1999] for convex, binary MINLP:

$$\underset{\eta, x}{\text{minimize}}\ \eta \quad \text{s.t. } \eta \geq f(x),\ c(x) \leq 0,\ x \in X,\ x_i \in \{0,1\}\ \forall\, i \in I$$

Node in BnB tree with solution x', and $0 < x'_j < 1$ for $j \in I$
Relaxation: $\mathcal{C} = \{x \in X \mid f(x) \leq \eta,\ c(x) \leq 0,\ 0 \leq x_I \leq 1\}$
Let $I_0, I_1 \subseteq I$ index sets of 0-1 vars fixed to zero or one

Goal: Generate a valid inequality tat cuts off x'
Consider two disjoint sets ("feasible sets after branching on x_j")

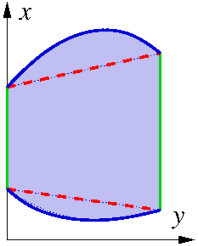
$$\mathcal{C}_j^0 = \{x \in \mathcal{C} \mid x_j = 0,\ 0 \leq x_i \leq 1\ \forall i \in I, i \neq j\},$$
$$\mathcal{C}_j^1 = \{x \in \mathcal{C} \mid x_j = 1,\ 0 \leq x_i \leq 1\ \forall i \in I, i \neq j\}.$$

... and find description of convex hull: $\tilde{M}_j(\mathcal{C}) = \text{conv}(\mathcal{C}_j^0 \cup \mathcal{C}_j^1)$

Disjunctive Cuts for MINLP

Extension of disjunctive cuts from MILP, [Balas, 1979]
Continuous relaxation

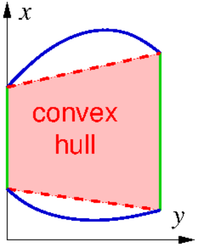
- $\mathcal{C} := \{x | c(x) \leq 0,\ 0 \leq x_I \leq 1,\ 0 \leq x_C \leq U\}$



Disjunctive Cuts for MINLP

Extension of disjunctive cuts from MILP, [Balas, 1979]
Continuous relaxation

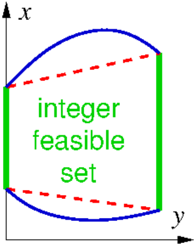
- $\mathcal{C} := \{x | c(x) \le 0,\ 0 \le x_I \le 1,\ 0 \le x_C \le U\}$
- $\mathcal{C} := \text{conv}(\{x \in \mathcal{C} \mid x_I \in \{0,1\}^p\})$



Disjunctive Cuts for MINLP

Extension of disjunctive cuts from MILP, [Balas, 1979]
Continuous relaxation

- $\mathcal{C} := \{x | c(x) \leq 0,\ 0 \leq x_I \leq 1,\ 0 \leq x_C \leq U\}$
- $\mathcal{C} := \text{conv}(\{x \in \mathcal{C} \mid x_I \in \{0,1\}^p\})$
- $\mathcal{C}_j^{0/1} := \{x \in \mathcal{C} | x_j = 0/1\}$



$$\text{let } \mathcal{M}_j(C) := \left\{ \begin{array}{l} z = \lambda_0 u_0 + \lambda_1 u_1 \\ \lambda_0 + \lambda_1 = 1,\ \lambda_0, \lambda_1 \geq 0 \\ u_0 \in \mathcal{C}_j^0,\ u_1 \in \mathcal{C}_j^1 \end{array} \right\}$$

$\Rightarrow \mathcal{P}_j(\mathcal{C}) :=$ projection of $\mathcal{M}_j(\mathcal{C})$ onto z

$\Rightarrow \mathcal{P}_j(\mathcal{C}) = \text{conv}\left(\mathcal{C} \cap x_j \in \{0,1\}\right)$ and $\mathcal{P}_{1\ldots p}(\mathcal{C}) = \mathcal{C}$

Disjunctive Cuts

Snag: Description of convex hull is nonconvex:

$$\text{let } \mathcal{M}_j(\mathcal{C}) := \left\{ \begin{array}{l} z = \lambda_0 u_0 + \lambda_1 u_1 \\ \lambda_0 + \lambda_1 = 1,\ \lambda_0, \lambda_1 \geq 0 \\ u_0 \in \mathcal{C}_j^0,\ u_1 \in \mathcal{C}_j^1 \end{array} \right\}$$

$\Rightarrow$ need global optimization solvers for separation problem

$\Rightarrow$ prohibitive; instead use convex formulation: $\tilde{M}_j(\mathcal{C})$

Disjunctive Cuts

Can describe $\tilde{M}_j(\mathcal{C})$ with perspective $\mathcal{P}_{c_i}$

$$\tilde{M}_j(\mathcal{C}) = \left\{ (x_F, v_0, v_1, \lambda_0, \lambda_1) \left| \begin{array}{ll} v_0 + v_1 = x_F, & v_{0j} = 0, \;\; v_{1j} = \lambda_1 \\ \lambda_0 + \lambda_1 = 1, & \lambda_0, \lambda_1 \geq 0 \\ \lambda_0 c_i(v_0/\lambda_0) \leq 0, 1 \leq \;\; i \leq m & \\ \lambda_1 c_i(v_1/\lambda_1) \leq 0, 1 \leq \;\; i \leq m & \end{array} \right. \right\},$$

Obtain a convex separation NLP ...

Disjunctive Cuts: Separation NLP

Goal: Find $\hat{x}$ closest to fractional solution x' in convex hull

$$\text{BC-SEP}(x', j) \begin{cases} \underset{x, v_0, v_1, \lambda_0, \lambda_1}{\text{minimize}} & ||x - x'||, \\ \text{subject to} & (x, v_0, v_1, \lambda_0, \lambda_1) \in \tilde{M}_j(\mathcal{C}) \\ & x_i = 0, \ \forall i \in I_0 \\ & x_i = 1, \ \forall i \in I_1. \end{cases}$$

optimal solution $\hat{x}$ with multipliers π_F for equality $v_0 + v_1 = x_F$

Theorem

Optimal dual solution of (BC-SEP(x', j)), then following cut is valid and eliminates x':

$$\pi_F^T x_F \leq \pi_F^T \hat{x}_F$$

Disjunctive Cuts: Example

Consider following MINLP example

$$\begin{cases} \underset{x_1,x_2}{\text{minimize}} & x_1 \\ \text{subject to} & (x_1 - \frac{1}{2})^2 + (x_2 - \frac{3}{4})^2 \le 1 \\ & -2 \le x_1 \le 2 \\ & x_2 \in \{0,1\} \end{cases}$$

$\Rightarrow$ solution of NLP relaxation: $x' = (x'_1, x'_2) = (-\frac{1}{2}, \frac{3}{4})$

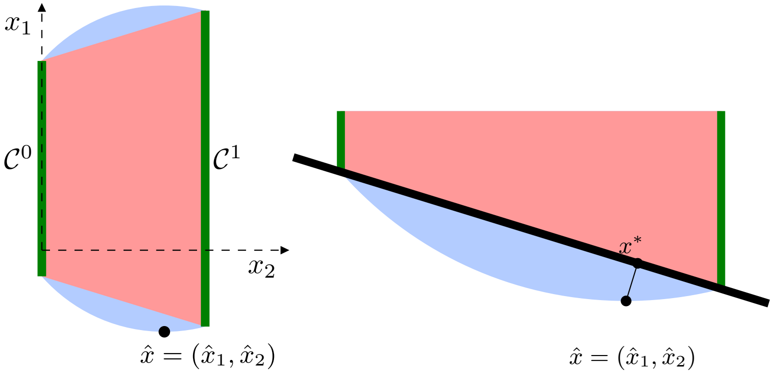
Solve $(x_1 - \frac{1}{2})^2 + (x_2 - \frac{3}{4})^2 \le 1$ for x_1, given $x_2 = 0$ and $x_2 = 1$:

$$\mathcal{C}^0 = \left\{ (x_1, 0) \in \mathbb{R} \times \{0,1\} \;\middle|\; 2 - \sqrt{7} \le 4x_1 \le 2 + \sqrt{7} \right\},$$

$$\mathcal{C}^1 = \left\{ (x_1, 1) \in \mathbb{R} \times \{0,1\} \;\middle|\; 2 - \sqrt{15} \le 4x_1 \le 2 + \sqrt{15} \right\}.$$

Solving (BC-SEP$(x', 2)$), we find the cut $x_1 + 0.3x_2 \ge -0.166$

Disjunctive Cuts: Example



Convex hull, relaxation, and disjunctive cut

Lifting Disjunctive Cuts

Cuts are only valid for sub-tree rooted at relaxation
To obtain globally valid cut

$$\pi^T x \leq \pi^T \hat{x}$$

assign

$$\pi_i = \min\{e_i^T H_0^T \mu_0, e_i^T H_1^T \mu_1\}, \; i \notin F$$

where e_i is i^{th} unit vector, F set of "free" variables and

- $\mu_0 = (\mu_{0F}, 0)$ and μ_{0F} multiplier of perspective $\mathcal{P}_c(v_0, \lambda_0) \leq 0$
- $\mu_1 = (\mu_{1F}, 0)$ and μ_{1F} multiplier of perspective $\mathcal{P}_c(v_1, \lambda_1) \leq 0$
- H_0, H_1 matrices of subgradient rows $\partial_v \mathcal{P}_{c_i}(v_j, \lambda_j)^T$, for $j = 0, 1$

Preferred norm for cut generation, (BC-SEP(x', j)), is ℓ_∞-norm

Outline

Implementation of Disjunctive Cuts

NLP (BC-SEP(x', j)) is not easy to solve:

- NLP has twice number of variables as original problem
- Perspective functions not differentiable at origin
- Hessian of perspective blows up near origin

$\Rightarrow$ NLP slow (and solvers may fail)

Suggest LP-based separation [Kılınç et al., 2010]

- Consider outer approximation relaxations of MINLP
- Iteratively tighten the outer approximation

$\Rightarrow$ faster and more robust cut generation

Implementation of Disjunctive Cuts

Let $\mathcal{B} \supset \mathcal{C} = \{x \in X \mid f(x) \leq \eta,\ c(x) \leq 0,\ 0 \leq x_I \leq 1\}$

Instead of $\mathcal{C}_j^0$ and $\mathcal{C}_j^1$ we consider

$$\mathcal{B}_j^0 = \{x \in \mathcal{B}^0 \mid x_j = 0\}, \quad \mathcal{B}_j^1 = \{x \in \mathcal{B}^0 \mid x_j = 1\}$$

valid inequalities for $\mathrm{conv}(\mathcal{B}_j^0 \cup \mathcal{B}_j^1)$ are also valid for $\mathrm{conv}(\mathcal{C}_j^0 \cup \mathcal{C}_j^1)$

Create linear (OA) sets $\mathcal{B}_j^0, \mathcal{B}_j^1$ iteratively (t):

$$\begin{aligned}\mathcal{B}_j^0(t) = \{x \in \mathbb{R}^n \mid x_j = 0,\ & f' + \nabla f'^T (x - x') \leq \eta, \\ & c' + \nabla c'^T (x - x') \leq 0,\ \forall x' \in \mathcal{K}_j^0(t)\},\end{aligned}$$

where $\mathcal{K}_j^0(t)$ set of linearization points; $\mathcal{B}_j^1(t)$ defined similarly

- $\mathcal{K}_j^0(t)$ augmented by solution of linear separation, x_t'
- Use "friendly points", $x_t' = \lambda x_{t0}' + (1 - \lambda) x_{t1}'$ for $\lambda \in [0, 1]$

$\Rightarrow$ converges to solution of (BC-SEP(x', j)); but slowly (?)

Outline

Summary and Exercises

Key points

- Single-tree methods are state-of-the-art
- Presolve for MINLP important ... need computational graph
- Branch-and-cut approaches being developed for MINLP

Solution to exercises ...

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