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

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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.

A2 (convexity) most restrictive (relaxed next week);
A3 is technical (MFCQ would have been sufficient);

Overview of Basic Methods

Two broad classes of method

1. Single-tree methods; e.g.
   - Nonlinear branch-and-bound
   - LP/NLP-based branch-and-bound
   - Nonlinear branch-and-cut

   ... build and search a single tree
2. Multi-tree methods; e.g.
   - Outer approximation
   - Benders decomposition
   - Extended cutting plane method

   ... alternate between NLP and MILP solves

Multi-tree methods only evaluate functions at integer points

Concentrate on methods for convex problems today.

Can mix different methods & techniques.

Outline

Nonlinear Branch-and-Bound

Solve NLP relaxation (x_I continuous, not integer)

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

- 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:

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

NLP relaxation is NLP$(-\infty, \infty)$

Nonlinear Branch-and-Bound

Branching: solution x' of (NLP(l,u)) feasible but not integral:

- Find a nonintegral variable, say $x'_i, i \in I$.
- Introduce two child nodes with bounds $(l^-, u^-) = (l^+, u^+) = (l, u)$ and setting:

$$u_i^- := \lfloor x'_i \rfloor, \quad \text{and} \quad l_i^+ := \lceil x'_i \rceil$$

- Two new NLPs: NLP(l^-, u^-) / NLP(l^+, u^+)
  ... corresponding to down/up branch

In practice, store problems on a heap $\mathcal{H}$

... pruning rules limit the tree $\Rightarrow$ no complete enumeration

Nonlinear Branch-and-Bound

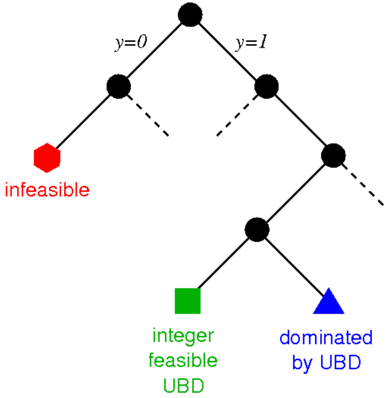
Pruning Rules: Let U upper bound on solution

- Infeasible: (NLP(l, u)) infeasible
  $\Rightarrow$ any NLP in subtree is also infeasible.
- Integer feasible: solution $x^{(l,u)}$ of (NLP(l, u)) integral
  - If $f(x^{(l,u)}) < U$, then new $x^* = x^{(l,u)}$ and $U = f^{(l,u)}$.
  - Otherwise, prune node: no better solution in subtree
- Dominated by U: optimal value of (NLP(l, u)), $f(x^{(l,u)}) \geq U$
  $\Rightarrow$ prune node: no better integer solution in subtree

Nonlinear Branch-and-Bound

Solve relaxed NLP ($0 \leq y \leq 1$ continuous relaxation)
. . . solution value provides lower bound

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



Search until no unexplored nodes
Software:

- GAMS-SBB, MINLPBB [L]
- BARON [Sahinidis] global
- Couenne [Belotti] global

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

Nonlinear Branch-and-Bound

BnB is finite, provided X is bounded polyhedron:

Theorem (Finiteness of Nonlinear BnB)

Solve MINLP by nonlinear branch-and-bound, and assume that A1-A3 hold. Then BnB terminates at optimal solution (or indication of infeasibility) after a finite number of nodes.

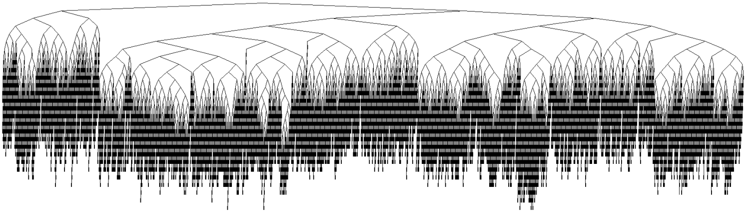
Proof.

- (A1-A3) $\Rightarrow$ every NLP solved globally
- Boundedness of X $\Rightarrow$ tree is finite

$\Rightarrow$ convergence, see e.g. Theorem 24.1 of [**?**]. □

Nonlinear Branch-and-Bound

BnB trees can get pretty large ...



Synthesis MINLP B&B Tree: 10000+ nodes after 360s

... be smart about solving NLPs & searching tree!

Outline

Advanced Nonlinear BnB

Basic BnB will work, but needs improvements:

- Selection of branching variables
- Node selection strategies
- Inexact NLP solves & hot-starts
- Cutting planes & branch-and-cut
- Software design & modern solvers, e.g. MINOTAUR

... critical for efficient implementation

Advanced Nonlinear BnB: Variable Selection

Ideally choose branching sequence to minimize tree size
... impossible in practice; sequence not known a priori
$\Rightarrow$ choose variable that maximizes increase in lower bound

Let $I_c \subset I$ set of fractional integer variables
... in practice choose subset of important variables (priorities)

Maximum Fractional Branching

Branch on variable i_0 with largest integer violation:

$$i_0 = \underset{i \in I_c}{\operatorname{argmax}} \left\{ \min \left(x_i - \lfloor x_i \rfloor \,,\, \lceil x_i \rceil - x_i \right) \right\},$$

... as bad as random branching [**?**]

Advanced Nonlinear BnB: Variable Selection

Successful rules estimate change in lower bound after branching

- Increasing lower bound improves pruning
- For $x_i, i \in I$, define degradation estimates D_i^+ and D_i^- for increase in lower bound
- Goal: make *both* D_i^+ and D_i^- large!
- Combine D_i^+ and D_i^- into single score:

$$s_i := \mu \min(D_i^+, D_i^-) + (1 - \mu) \max(D_i^+, D_i^-),$$

where parameter $\mu \in [0, 1]$ close to 1.

Degradation-Based Branching

Branch on variable i_0 with largest integer violation:

$$i_0 = \underset{i \in I_c}{\operatorname{argmax}} \{s_i\}$$

... methods differ by how D_i^+ and D_i^- computed

Advanced Nonlinear BnB: Variable Selection

The first approach for computing degradations is ...

Strong Branching

Solve $2 \times |I_c|$ NLPs for every potential child node:

- Solution at current (parent) node (NLP(l, u)) is $f_p := f^{(l,u)}$
- $\forall\, x_i, i \in I_c$ create two temporary NLPs: NLP$_i(l^-, u^-)$ and NLP$_i(l^+, u^+)$
- Solve both NLPs ...
  ... if both infeasible, then prune (NLP(l, u))
  ... if one infeasible, then fix integer in parent (NLP(l, u))
  ... otherwise, let solutions be f_i^+ and f_i^- and compute

$$D_i^+ = f_i^+ - f_p, \quad \text{and} \quad D_i^- = f_i^- - f_p.$$

Advanced Nonlinear BnB: Variable Selection

Advantage/Disadvantage of strong branching:

- Good: Reduce the number of nodes in tree
- Bad: Slow overall, because too many NLPs solved
- Solving NLPs approximately does not help

Fact: MILP $\neq$ MINLP

LPs hot-start efficiently (re-use basis factors),
but NLPs cannot be warm-started (neither IPM nor SQP)!

Reason (NLPs are, well ... nonlinear):

- NLP methods are iterative: generate sequence $\{x^{(k)}\}$
- At solution, $x^{(l)}$, have factors from $x^{(l-1)}$ ... out-of-date

Approximate Strong Branching

Simple idea: Use QP (LP) approximation [?]

CPU[s] for root node and round (2 # ints) of strong branching:

problem	# ints	Full NLP	Cold QP	Hot QP
stockcycle	480	4.08	3.32	0.532
RSyn0805H	296	78.7	69.8	1.94
SLay10H	180	18.0	17.8	1.25
Syn30M03H	180	40.9	14.7	2.12

- Small savings from replacing NLP by QP solves.
- Order of magnitude saving from re-using factors.

Approximate Strong Branching

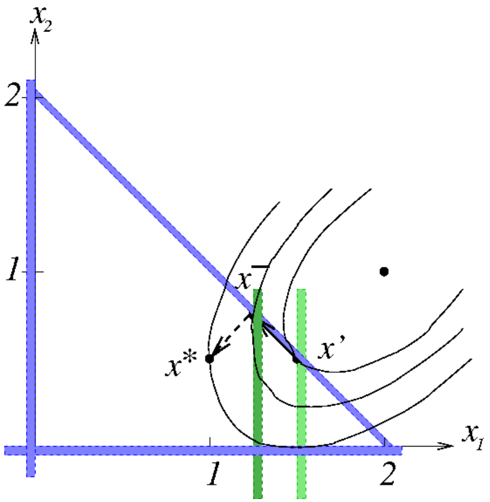
Hot-QP Starts in BQPD [Fletcher]

- parent node is dual feasible after branching
- perform steps of dual active-set method to get primal feasible
- re-use factors of basis $B = LU$
- re-use factors of dense reduced Hessian $Z^T HZ = L^T DL$
- use LU and $L^T DL$ to factorize KKT system

$$\begin{bmatrix} H & A^T \\ A & 0 \end{bmatrix} \quad \text{where} \quad B^{-1} = [A : V]^{-1} = \begin{bmatrix} Y \\ Z \end{bmatrix}$$

- 2-3 pivots to re-optimize independent of problem size

Approximate Strong Branching



Parametric QP solve

Performance Profiles [Dolan and More, 2002]

name	Random CPU	Random nodes	Most-Fractional CPU	Most-Fractional nodes
BatchS101006M	141.9	9464	68.7	7560
BatchS121208M	2694.8	96566	566.1	41600
BatchS151208M	6781.6	176188	1710.0	102744
BatchS201210M	> 10800	> 174400	6050.6	275740
CLay0204H	61.0	4272	27.3	3404
CLay0204M	7.0	4563	0.7	1361
CLay0205H	[illegible]271.9	104[illegible]2	205[illegible]	81922
CLay0205M	338.[illegible]	99[illegible]4	2[illegible]	22695
CLay0303M	[illegible]	[illegible]22	[illegible]	1032
CLay0304H	48[illegible]9	24[illegible]44	137[illegible]9	11631
CLay0304M	7[illegible]	28[illegible]4	4[illegible]	30698
CLay0305H	7160.[illegible]	160[illegible]83	2169.1	70552
CLay0305M	710.9	185254	56.7	38282
FLay04H	49.3	3158	37.1	3012
FLay04M	1.9	3294	1.4	2504
FLay05H	8605.9	185954	4781.3	129598
FLay05M	215.2	188346	125.3	114122
FLay06M	> 10800	> 5166800	> 10800	> 6022600

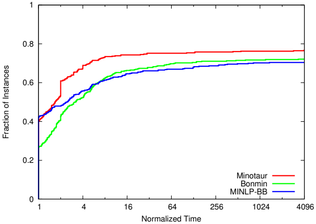
No!!!

Performance profiles
Clever way to display a benchmark

$$\forall \text{ solver } s \quad \log_2\left(\frac{\#\ \text{iter}(s,p)}{\text{best\_iter}(p)}\right)$$

$$p \in \text{problem}$$

- "probability distribution": solver "A" is at most x-times slower than best.
- Origin shows percentage of problems where solver "A" is best.
- Asymptotics shows reliability of solver "A".



Performance Profiles (Formal Definition)

Performance ratio of $t_{p,s}$ for $p \in \mathcal{I}$ of problems, $s \in S$ of solvers:

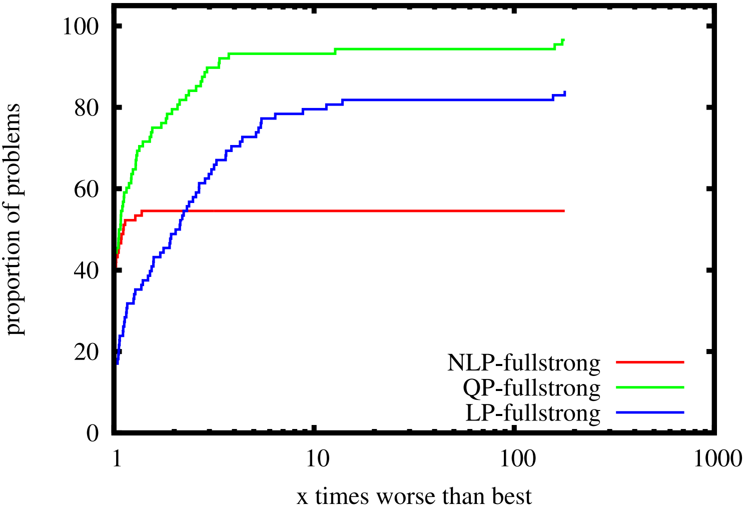
$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,i} \mid i \in S,\}}$$

distribution function $\rho_s(\tau)$ for solver $s \in S$

$$\rho_s(\tau) = \frac{\text{size}\{p \in \mathcal{I} \mid r_{p,s} \leq \tau\}}{|\mathcal{I}|}.$$

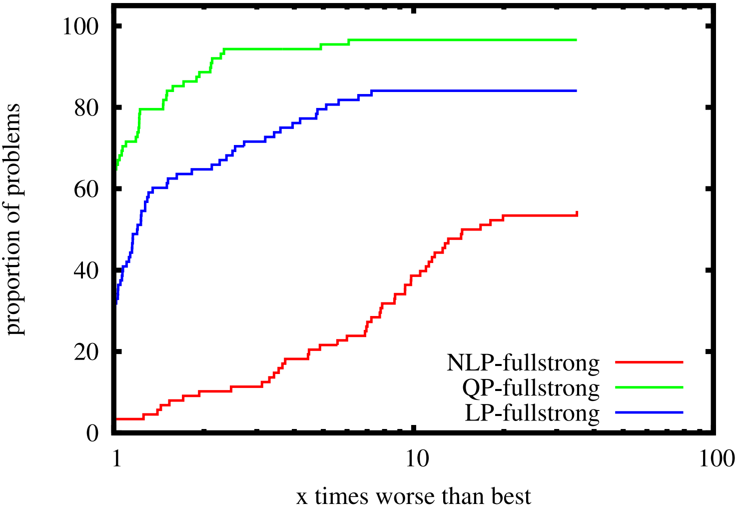
$\rho_s(\tau)$ probability that solver s is at most $\tau\times$ slower than best

Approximate Strong Branching



Performance (# nodes) of NLP/QP/LP strong branching

Approximate Strong Branching



Performance (CPU time) of NLP/QP/LP strong branching

Advanced Nonlinear BnB: Variable Selection

Pseudocost Branching

Keep history of past branching to estimate degradations

- n_i^+, n_i^- number of times up/down node solved for variable i
- p_i^+, p_i^- pseudocosts updated when child solved:

$$p_i^+ = \frac{f_i^+ - f_p}{\lceil x_i \rceil - x_i} + p_i^+, \; n_i^+ = n_i^+ + 1 \;\; \text{or} \;\; p_i^- = \ldots \; n_i^- = \ldots$$

- Compute estimates of D_i^+ and D_i^- or branching:

$$D_i^+ = (\lceil x_i \rceil - x_i) \frac{p_i^+}{n_i^+} \;\; \text{and} \;\; D_i^- = (x_i - \lfloor x_i \rfloor) \frac{p_i^-}{n_i^-}.$$

- Initialize pseudocosts with strong branching
- Good estimates for MILP, [**?**]
- Not clear how to update, if NLP infeasible ... ℓ_1 penalty?

Advanced Nonlinear BnB: Variable Selection

Following approach combines strong branching and pseudocosts

Reliability Branching

Strong branching early, then pseudocost branching

- While n_i^+ or $n_i^- \leq \tau (= 5)$ do strong branching on x_i
- Once n_i^+ or $n_i^- > \tau$ switch to pseudocost

Important alternatives to variables branching:

- SOS branching, see [**?**]
- Branching on split disjunctions

$$\left(a^T x_I \leq b\right) \vee \left(a^T x_I \geq b + 1\right)$$

where $a \in \mathbb{Z}^p$ and $b \in \mathbb{Z}$ ... conceptually like conjugate directions

Advanced Nonlinear BnB: Node Selection

Strategic decision on which node to solve next.

Goals of node selection

- Find good feasible solution quickly to reduce upper bound, U
- Prove optimality of incumbent x^* by increasing lower bound

Popular strategies:

1. Depth-first search
2. Best-bound search
3. Hybrid schemes

Advanced Nonlinear BnB: Depth-First Search

Depth-First Search

Select deepest node in tree (or last node added to heap $\mathcal{H}$)

Advantages:

- Easy to implement (Sven likes that ;-)
- Keeps list of open nodes, $\mathcal{H}$, as small as possible
- Minimizes the change to next NLP (NLP(l, u)):
  ... only single bound changes $\Rightarrow$ better hot-starts

Disadvantages:

- poor performance if no upper bound is found:
  $\Rightarrow$ explores nodes with a lower bound larger than solution

Advanced Nonlinear BnB: Best-Bound Search

Best-Bound Search

Select node with best lower bound

Advantages:

- Minimizes number of nodes for fixed sequence of branching decisions, because all explored nodes would have been explored independent of upper bound

Disadvantages:

- Requires more memory to store open problems
- Less opportunity for warm-starts of NLPs
- Tends to find integer solutions at the end

Advanced Nonlinear BnB: Best-Bound Search

1. Best Expected Bound: node with best bound after branching:

$$b_p^+ = f_p + (\lceil x_i \rceil - x_i)\frac{p_i^+}{n_i^+} \quad \text{and} \quad b_p^- = f_p + (x_i - \lfloor x_i \rfloor)\frac{p_i^-}{n_i^-}.$$

   Next node is $\max_p \left\{ \min \left(b_p^+, b_p^- \right) \right\}$.

2. Best Estimate: node with best expected solution in subtree

$$e_p = f_p + \sum_{i: x_i \text{fractional}} \min \left((\lceil x_i \rceil - x_i)\frac{p_i^+}{n_i^+} , \; (x_i - \lfloor x_i \rfloor)\frac{p_i^-}{n_i^-} \right),$$

   Next node is $\max_p \{ e_p \}$.

... good search strategies combine depth-first and best-bound

Advanced Nonlinear BnB: Inexact NLP Solves

Role for inexact solves in MINLP

- Provide approximate values for strong branching
- Solve NLPs inexactly during tree-search:
  - [?] consider single SQP iteration
    ... perform early branching if limit seems non-integral
    ... augmented Lagrangian dual for bounds
  - [?] considers single SQP iteration
    ... use outer approximation instead of dual
    ... numerical results disappointing

  ... reduce solve time by factor 2-3 at best
- New idea: search QP tree & exploit hot-starts for QPs
  ... QP-diving discussed next ...

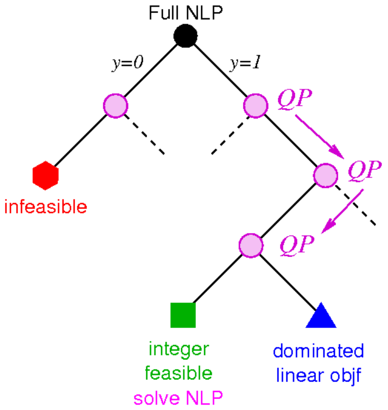
Advanced Nonlinear BnB: QP-Diving

Branch-and-bound solves huge number of NLPs ⇒ bottleneck!

QP-Diving Tree-Search:

- solve root node & save factors from last QP solve
- same KKT for whole subtree
- perform MIQP tree-searches
  - depth-first search: ⇒ fast hot-starts
  - back-track: warm-starts

Need new fathoming rules ...



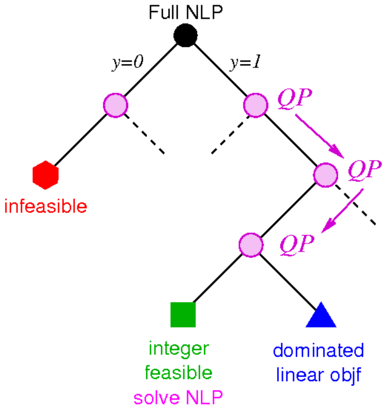
... alternative: change QP approximation after back-track

Advanced Nonlinear BnB: QP-Diving

Assume MINLP is convex

QP-Diving Tree-Search:
Solve QPs until

1. QP infeasible: ●
   ... QP is relaxation of NLP
2. Node integer feasible: □
   $\Rightarrow$ NLP to get upper bnd (U)
   ... QP over-/under-estimates
   $\Rightarrow$ resolve
3. Infeasible O-cut $\eta < U$: ▲
   Linear O-cut: $\eta \geq f_k + g_k^T d$



New Extended Performance Profiles

Performance ratio of $t_{p,s}$ for $p \in \mathcal{I}$ of problems, $s \in S$ of solvers:

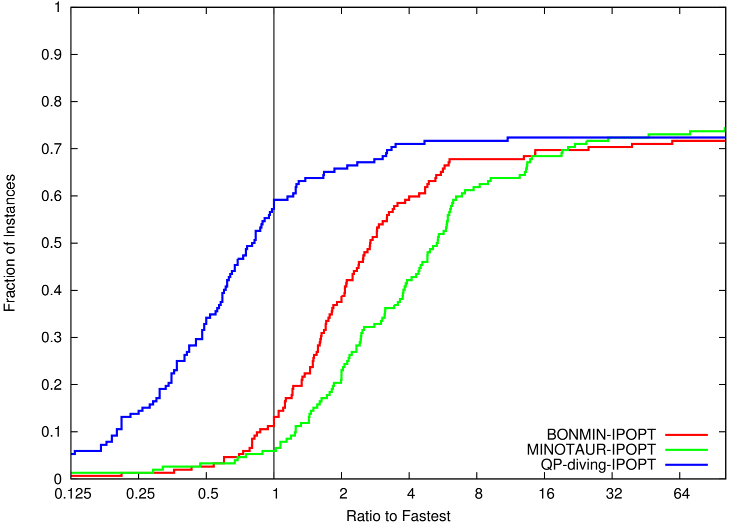
$$\hat{r}_{p,s} = \frac{t_{p,s}}{\min\{t_{p,i} \mid i \in S, i \neq s\}}$$

distribution function $\rho_s(\tau)$ for solver $s \in S$

$$\hat{\rho}_s(\tau) = \frac{\text{size}\{p \in \mathcal{I} \mid \hat{r}_{p,s} \leq \tau\}}{|\mathcal{I}|}.$$

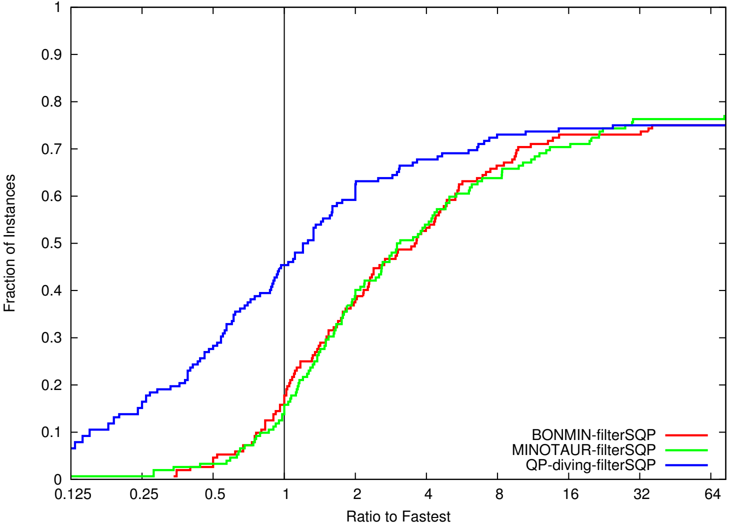
- $\hat{\rho}_s(\tau)$ probability that solver s is at most $\tau\times$ slower than best
- For $\hat{r}_{p,s} \geq 1$ get standard performance profile
- Extension: $\hat{r}_{p,s} < 1$ if solver s is fastest for instance p
- $\hat{\rho}_s(0.25)$ probability that solver s is $4\times$ faster than others

CPU-Times for MINOTAUR with Hot-Starts (IPOPT)



Hot-started QP give a huge improvement

CPU-Times for MINOTAUR with Hot-Starts (filterSQP)



Hot-started QP give a huge improvement

Typical Results

RSyn0840M02M

Solver	CPU	NLPs	CPU/100NLPs
IPOPT	7184.91	69530	10.3335
filterSQP	7192.54	37799	19.0284
QP-Diving	5276.23	1387837	0.3802

$\Rightarrow$ many more nodes ... a little faster.

CLay0305H

Solver	CPU	NLPs	CPU/100NLPs
IPOPT	1951.1	16486	11.8349
filterSQP	849.74	16717	5.0831
QP-Diving	97.89	24029	0.4074

$\Rightarrow$ similar number of nodes ... much faster!

MINOTAUR: A New Software Framework for MINLP

Mixed
Integer
Nonlinear
Optimization
Toolkit:
Algorithms,
Underestimators &
Relaxations

It's only half bull

Goal: Implement a Range of Algorithms in Common Framework

- Fast, usable MINLP solver.
- Flexibility for developing new algorithms.
- Ease of developing new algorithms.

MINOTAUR's Four Main Components

Interfaces for reading input

- AMPL

Engines to solve LP/NLP/QP

- QP: BQPD
- NLP: FilterSQP/IPOPT
- LP: OSI-CLP

Algorithms to solve MINLP

- Branch-and-Bound
- Outer-Approximation
- Quesada-Grossmann
- Branch-and-Refine

Base

- Data Structures:
  - Problem
  - Objective & Constraints
  - Functions
  - Modifications
  - Gradient, Jacobian, Hessian
- Tools for Search:
  - Node Processors
  - Node Relaxers
  - Branchers
  - Tree Manager
- Utilities
  - Loggers & Timers
  - Options

MINOTAUR's Four Main Components

Interfaces for reading input

- AMPL
- Your Interface Here

Engines to solve LP/NLP/QP

- QP: BQPD
- NLP: FilterSQP/IPOPT
- LP: OSI-CLP
- Your engine here

Algorithms to solve MINLP

- Branch-and-Bound
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Base

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- Your Tools for Search:
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  - Node Relaxers
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- Utilities
  - Loggers & Timers
  - Options

Highly Customizable

MINOTAUR Approach to MINLP: Handlers

- Branch-and-$\{$Bound$\|$Cut$\|$Reduce$\}$ alg^s require methods to
  - Relax a problem
  - Reformulate a problem
  - Presolve a problem
  - Check feasibility of a given point
  - Separate a given point
  - Find a branching candidate
  - Branch on a candidate

... methods depend on structure of constraints or objective

MINOTAUR Approach to MINLP: Handlers

- Branch-and-$\{$Bound$\|$Cut$\|$Reduce$\}$ alg^s require methods to
  - Relax a problem
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  - Separate a given point
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  ... methods depend on structure of constraints or objective
- Handlers implement (type specific) above methods

  ... adopted from constraint-programming solver: SCIP
- MINOTAUR's Handlers:
  - IntVarHandler
  - LinearHandler
  - BilinearHandler
  - MultilinearHandler, ...
- Branch-and-xxx components like Nodeprocessor, Brancher can be agnostic to type of objective and constraints.

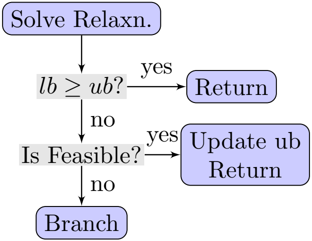
MINLP Branch-and-Bound in MINOTAUR

How to write an NLP Branch-and-Bound solver in MINOTAUR:

Node Relaxer

Do nothing!

Node Processor



Brancher

Pick a fractional variable.

Use Minotaur::IntVarHandler for all three

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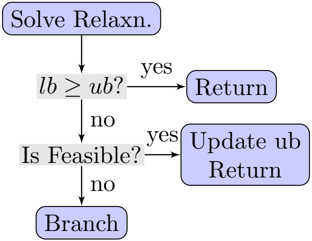

Brancher

Pick a fractional variable.

Use Minotaur::IntVarHandler for all three

```
relax() {
// empty
}
```

```
bool isFeasible() {
// test integrality
}
```

```
cand* findBrCandidates() {
// return fractional vars
}
branch(cand) {
// return modifications
}
```

MINLP Branch-and-Bound in MINOTAUR

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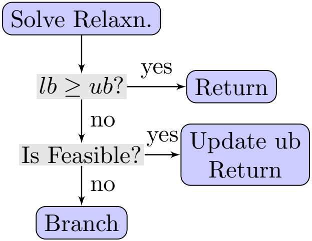
Do nothing!

Node Processor



Brancher

Pick a fractional variable.

Use Minotaur::IntVarHandler for all three

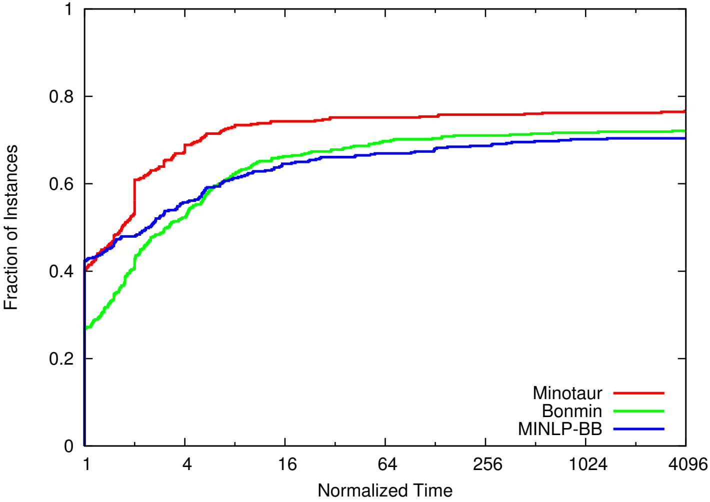
Solver in < 200 lines:

- Read instance. Load Engine.
- Create IntVarHandler.
- Load it to NodeProcessor, Brancher, NodeRelaxer.
- Solve

Features

	Bonmin	FilMINT	BARON	Couenne	Minotaur
Algorithms:					
NLP B&B	✓	×	×	×	✓
Branch & Cut	✓	✓	×	×	✓
Branch & Reduce	×	×	✓	✓	✓
Support for Nonlinear Functions:					
Comput. Graph	×	×	✓	✓	✓
Nonlin. Reform.	×	×	×	×	✓
Native Derivat.	×	×	×	×	✓
Interfaces:					
AIMMS	×	×	✓	×	×
AMPL	✓	✓	×	✓	✓
GAMS	✓	×	✓	✓	×
Open Source	✓	×	×	✓	✓

MINOTAUR Performance



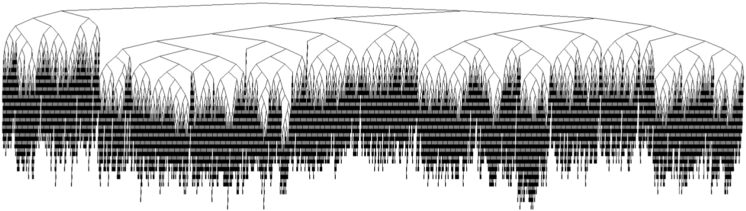
Time taken for 463 MINLP Instances from GAMS, MacMINLP, CMU test-sets.

MINOTAUR's Soft-Wear Stack

... available at www.mcs.anl.gov/minotaur

Outline

MINLP Trees are Huge



Synthesis MINLP B&B Tree: 10000+ nodes after 360s

$\Rightarrow$ use MILP solvers to search tree?

Multi-Tree Methods

MILP solvers much better developed than MINLP

- LPs are easy to hot-start
- Decades of investment into software
- MILPs much easier; e.g. no need for constraint qualifications

$\Rightarrow$ developed methods that exploit this technology

Multi-Tree Methods

- Outer approximation [**?**]
- Benders decomposition [**?**]
- Extended cutting plane method [**?**]

... solve a sequence of MILP (and NLP) problems

Multi-tree methods evaluate functions “only” at integer points!

Multi-Tree Methods

Recall the η-MINLP formulation

$$\begin{cases} \underset{\eta, x}{\text{minimize}} & \eta, \\ \text{subject to} & f(x) \leq \eta, \\ & c(x) \leq 0, \\ & x \in X, \\ & x_i \in \mathbb{Z}, \ \forall i \in I. \end{cases}$$

where we have "linearized" the objective: $\eta \geq f(x)$

Use η-MINLP in this section

Outer Approximation

Mixed-Integer Nonlinear Program (MINLP)

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

NLP subproblem for fixed integers $x_I^{(j)}$:

$$\text{NLP}(x_I^{(j)}) \begin{cases} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to } c(x) \le 0 \\ & x \in X \quad \text{and } x_I = x_I^{(j)}, \end{cases}$$

with solution $x^{(j)}$.

If $(\text{NLP}(x_I^{(j)}))$ infeasible then solve feasibility problem ...

Outer Approximation

Mixed-Integer Nonlinear Program (MINLP)

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

NLP feasibility problem for fixed integers $x_I^{(j)}$:

$$\mathrm{F}(x_I^{(j)}) \begin{cases} \underset{x}{\text{minimize}} & \displaystyle\sum_{i \in J^{\perp}} w_i c_i^{+}(x) \\ \text{subject to} & c_i(x) \leq 0,\; i \in J \\ & x \in X \quad \text{and } x_I = x_I^{(j)}, \end{cases}$$

where $w_i > 0$ are weights and solution is $x^{(j)}$.

$(\mathrm{F}(x_I^{(j)}))$ generalize minimum norm solution
... provides certificate that $(\mathrm{NLP}(x_I^{(j)}))$ infeasible

Outer Approximation

Convexity of f and c implies that

Lemma (Supporting Hyperplane)

Linearization about solution $x^{(j)}$ of $(NLP(x_I^{(j)}))$ or $(F(x_I^{(j)}))$,

$$(OA) \quad \eta \geq f^{(j)} + \nabla f^{(j)^T}(x - x^{(j)}) \quad \text{and} \quad 0 \geq c^{(j)} + \nabla c^{(j)^T}(x - x^{(j)}),$$

are outer approximations of the feasible set of η-MINLP.

Lemma (Feasibility Cuts)

If $(NLP(x_I^{(j)}))$ infeasible, then (OA) cuts off $x_I = x_I^{(j)}$.

Outer Approximation

Mixed-Integer Nonlinear Program (η-MINLP)

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

Define index set of all possible feasible integers, $\mathcal{X}$

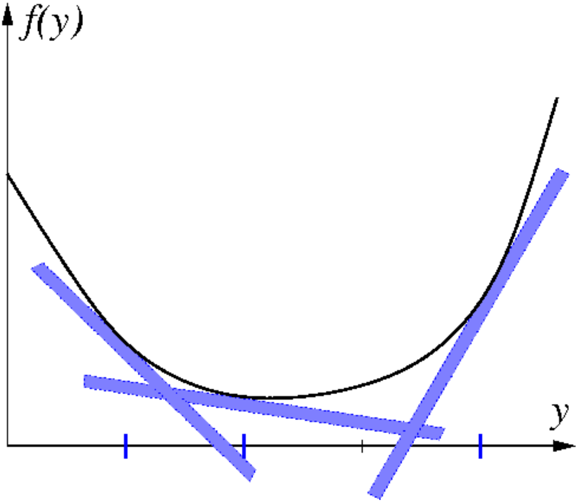
$$\mathcal{X} := \left\{ x^{(j)} \in X : x^{(j)} \text{ solves } (\text{NLP}(x_I^{(j)})) \quad \text{or } (\text{F}(x_I^{(j)})) \ \right\}.$$

... boundedness of X implies $|\mathcal{X}| < \infty$

Construct equivalent OA-MILP (outer approximation MILP)

$$\begin{cases} \underset{\eta, x}{\text{minimize}} & \eta, \\ \text{subject to} & \eta \geq f^{(j)} + \nabla f^{(j)^T}(x - x^{(j)}), \ \forall x^{(j)} \in \mathcal{X} \\ & 0 \geq c^{(j)} + \nabla c^{(j)^T}(x - x^{(j)}), \ \forall x^{(j)} \in \mathcal{X} \\ & x \in X, \\ & x_i \in \mathbb{Z}, \ \forall i \in I. \end{cases}$$

Outer Approximation in Less Than 1000 Words



Outer Approximation

Theorem (Equivalence of OA-MILP and MINLP)

Let assumptions A1-A3 hold

- *If x^* solves MINLP, then it also solves OA-MILP*
- *If (η^*, x^*) solves OA-MILP, then η^* is optimal value of MINLP, and x_I^* is an optimal integer.*

MILP and MINLP are not quite equivalent

Example where OA-MILP not equivalent to MINLP

$$\underset{x}{\text{minimize}} \; x_3 \quad \text{subject to} (x_1 - \tfrac{1}{2})^2 + x_2^2 + x_3^3 \leq 1, \; x_1 \in \mathbb{Z} \cap [-1, 2].$$

... OA-MILP has no coefficients for x_2 ... undefined

Outer Approximation Algorithm

Solving OA-MILP clearly not sensible; define upper bound as

$$U^k := \min_{j \le k} \left\{ f^{(j)} \mid (\text{NLP}(x_I^{(j)})) \text{ is feasible } \right\}.$$

Define relaxation of OA-MILP, using $\mathcal{X}^k \subset \mathcal{X}$, with $\mathcal{X}^0 = \{0\}$

$$M(\mathcal{X}^k) \begin{cases} \underset{\eta, x}{\text{minimize}} & \eta, \\ \text{subject to} & \eta \le U^k - \epsilon \\ & \eta \ge f^{(j)} + \nabla f^{(j)^T}(x - x^{(j)}), \ \forall x^{(j)} \in \mathcal{X}^k \\ & 0 \ge c^{(j)} + \nabla c^{(j)^T}(x - x^{(j)}), \ \forall x^{(j)} \in \mathcal{X}^k \\ & x \in X, \\ & x_i \in \mathbb{Z}, \ \forall i \in I. \end{cases}$$

... build up better OA $\mathcal{X}^k$ iteratively for $k = 0, 1, \ldots$

Outer Approximation Algorithm

Outer approximation

Given $x^{(0)}$, choose tol $\epsilon > 0$, set $U^{-1} = \infty$, set $k = 0$, and $\mathcal{X}^{-1} = \emptyset$.

repeat

  Solve (NLP($x_I^{(j)}$)) or (F($x_I^{(j)}$)); solution $x^{(j)}$.

  if *(NLP($x_I^{(j)}$)) feasible & $f^{(j)} < U^{k-1}$* **then**

    Update best point: $x^* = x^{(j)}$ and $U^k = f^{(j)}$.

  else

    Set $U^k = U^{k-1}$.

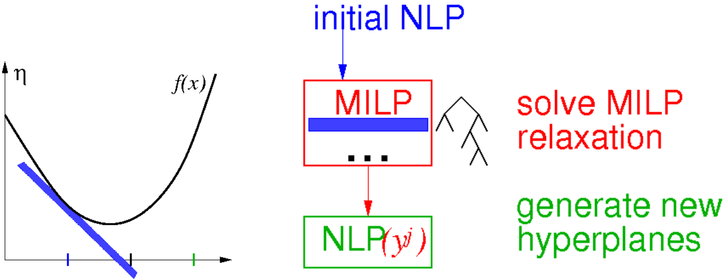
  Linearize f and c about $x^{(j)}$ and set $\mathcal{X}^k = \mathcal{X}^{k-1} \cup \{j\}$.

  Solve $(M(\mathcal{X}^k))$, let solution be $x^{(k+1)}$ & set $k = k + 1$.

until *MILP $(M(\mathcal{X}^k))$ is infeasible*

Outer Approximation Algorithm

Alternate between solve NLP(y_j) and MILP relaxation

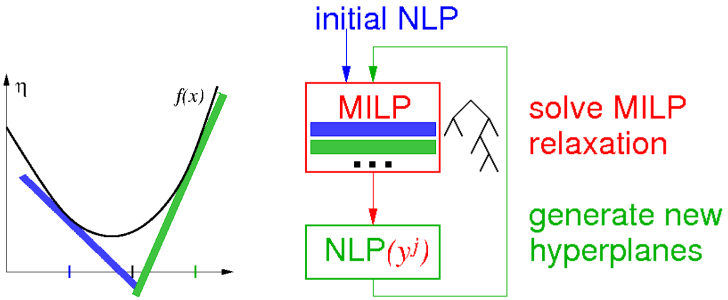


MILP $\Rightarrow$ lower bound; NLP $\Rightarrow$ upper bound

... convergence follows from convexity & finiteness

Outer Approximation Algorithm

Alternate between solve NLP(y_j) and MILP relaxation



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

... convergence follows from convexity & finiteness

Outer Approximation Algorithm

Theorem (Convergence of Outer Approximation)

Let Assumptions A1-A3 hold, then outer approximation terminates finitely at optimal solution of MINLP or indicates it is infeasible.

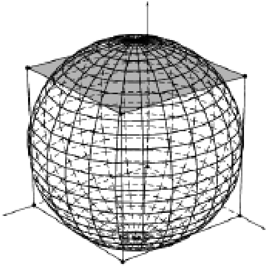
Outline of Proof.

- Optimality of $x^{(j)}$ in (NLP($x_I^{(j)}$))
  $\Rightarrow \eta \geq f^{(j)}$ for feasible point of $(M(\mathcal{X}^k))$
  ... ensures finiteness, since X compact
- Convexity $\Rightarrow$ linearizations are supporting hyperplanes
  ... ensures optimality

Worst Case Example of Outer Approximation

[?] construct infeasible MINLP:

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



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

Lemma

OA cannot cut more than one vertex of the hypercube
MILP master problem feasible for any $k < 2^n$ OA cuts

Theorem

OA visits all 2^n vertices

Benders Decomposition

Can derive Benders cut from outer approximation:

- Take optimal multipliers $\lambda^{(j)}$ of (NLP($x_I^{(j)}$))
- Sum outer approximations

$$
\begin{array}{rrl}
 & \eta \geq & f^{(j)} + \nabla f^{(j)^T}(x - x^{(j)}) \\
+ \quad \lambda^{(j)^T} (& 0 \geq & c^{(j)} + \nabla c^{(j)^T}(x - x^{(j)}) \;) \\
\hline
 & \eta \geq & f^{(j)} + \nabla_I \mathcal{L}^{(j)^T}(x_I - x_I^{(j)})
\end{array}
$$

- Using KKT conditions wrt continuous variables x_C:
  $0 = \nabla_C \mathcal{L}^{(j)} = \nabla_C f + \nabla_C c \lambda^{(j)}$ & $\lambda^{(j)^T} c^{(j)} = 0$
  ... eliminates continuous variables, x_C

Benders cut only involves integer variables x_I.
Can write cut as $\eta \geq f^{(j)} + \mu^{(j)^T}(x_I - x_I^{(j)})$,
where $\mu^{(j)}$ multiplier of $x = x_I^{(j)}$ in (NLP($x_I^{(j)}$))

Benders Decomposition

For MINLPs with convex problems functions f, c, we can show:

1. Benders cuts are weaker than outer approximation
   - Benders cuts are linear combination of OA
2. Outer Approximation & Benders converge finitely
   - Functions f, c convex $\Rightarrow$ OA cuts are outer approximations
   - OA cut derived at optimal solution to NLP subproblem
     $\Rightarrow \nexists$ feasible descend directions
     ... every OA cut corresponds to first-order condition
   - Cannot visit same integer $x_I^{(j)}$ more than once

   $\Rightarrow$ terminate finitely at optimal solution

Readily extended to situations where $(\text{NLP}(x_I^{(j)}))$ not feasible.

Extended Cutting Plane (ECP) Method

ECP is variation of OA

- Does not solve any NLPs
- Linearize f, c around solution of MILP, $x^{(k)}$:
  If $x^{(k)}$ feasible in linearization, then solved MINLP
  Otherwise, pick linearization violated by $x^{(k)}$ and add to MILP

Properties of ECP

- Convergence follows from OA & Kelley's cutting plane method
- NLP convergence rate is linear
- Can visit same integer more than once ...

... single-tree methods use ECP cuts to speed up convergence

Summary of Multi-Tree Methods

Three Classes of Multi-Tree Methods

1. Outer approximation based on first-order expansion
2. Benders decomposition linear combination of OA cuts
3. Extended cutting plane method: avoids NLP solves

Common Properties of Multi-Tree Methods

- Only need to solve final MILP to optimality
  ... can terminate MILP early ... adding more NLPs
- Can add cuts from incomplete NLP solves
- Worst-case example for OA also applies for Benders and ECP
- No warm-starts for MILP ... expensive tree-search

... motivates single-tree methods next ...

Outline

Summary and Exercises

Key points

- Single and multi-tree methods have advantages
- Exploit linearity (or QP) as much as possible
- Implementation matters ... many modern solvers

Exercise for Credit

Prepare a 2-5 minute short chat about why you are interested in MINLP. Present on Monday after the lecture. Email Sven to let him know that you will talk. You can (but do not have to) use slides.

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