

Convex Mixed-Integer Nonlinear Optimization I Summer School on Optimization of Dynamical Systems

Sven Leyffer and Jeff Linderoth

Argonne National Laboratory

September 3-7, 2018



Outline



- 2 Nonlinear Branch-and-Bound
- 3 Multi-Tree Methods



Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

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

Basic Assumptions for Convex MINLPA1 \mathcal{X} is a bounded polyhedral set.A2 f and c twice continuously differentiable convexA3 MINLP satisfies a constraint qualification.

A2 (convexity) most restrictive (show how to relax later) A3 is technical (MFCQ would have been sufficient)

Overview of Basic Methods

Two broad classes of method

- 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
- Ø 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.

Overview of Components of Methods

All MINLP solvers built on following components ... Relaxation

- Used to compute a lower bound on the optimum
- Obtained by enlarging feasible set; e.g. ignore constraints
- Typically much easier to solve than MINLP

Constraint Enforcement

- Exclude solutions from relaxations not feasible in MINLP
- Refine or tighten of relaxation; e.g. add valid inequalities

Upper Bounds

• Obtained from any feasible point; e.g. solve NLP for fixed $x_{\mathcal{I}}$

Outline of Relaxations



Nonlinear and polyhedral relaxation

Theorem (Relaxation Property)

If solution of relaxation is feasible, then it is optimal.

Relaxations of Integrality

Definition (Relaxation)

Optimization problem min{ $\check{f}(x) : x \in \mathcal{R}$ } is a relaxation of min{ $f(x) : x \in \mathcal{F}$ }, iff $\mathcal{R} \supset \mathcal{F}$ and $\check{f}(x) \leq f(x)$ for all $x \in \mathcal{F}$.

Goal: relaxation easy to solve globally, e.g. MILP or NLP

Relaxing Integrality

4

- Relax Integrality $x_i \in \mathbb{Z}$ to $x_i \in \mathbb{R}$ for all $i \in \mathcal{I}$
- Gives nonlinear relaxation of MINLP, or NLP:

$$\begin{cases} \underset{x}{\text{minimize } f(x),} \\ \text{subject to } c(x) \leq 0, \\ x \in \mathcal{X}, \text{ continuous} \end{cases}$$



Used in branch-and-bound algorithms

Relaxations of Nonlinear Convex Constraints

Relaxing Convex Constraints

Convex 0 ≥ c(x) and η ≥ f(x)f relaxed by supporting hyperplanes

$$\eta \ge f^{(k)} + \nabla f^{(k)^{T}}(x - x^{(k)}) \\ 0 \ge c^{(k)} + \nabla c^{(k)^{T}}(x - x^{(k)})$$

for a set of points $x^{(k)}$, $k = 1, \ldots, K$.

- Obtain polyhedral relaxation of convex constraints.
- Used in the outer approximation methods.



Constraint Enforcement

Goal: Given solution of relaxation, \hat{x} , not feasible in MINLP, exclude it from further consideration to ensure convergence

Three constraint enforcement strategies

- Relaxation refinement: tighten the relaxation
- Ø Branching: disjunction to exclude set of non-integer points
- Spatial branching: divide region into sub-regions

Strategies can be combined ...

Constraint Enforcement: Branching

Eliminate current \hat{x} solution by branch on integer variables:

- **()** Select fractional \hat{x}_i for some $i \in \mathcal{I}$
- Oreate two new relaxations by adding

 $x_i \leq \lfloor \hat{x}_i \rfloor$ and $x_i \geq \lceil \hat{x}_i \rceil$ respectively

... solution to MINLP lies in one of the new relaxations.



Constraint Enforcement: Refinement

Tighten the relaxation to remove current solution \hat{x} of relaxation

- Add a valid inequality to relaxation, i.e. an inequality that is satisfied by all feasible solutions of MINLP
- Valid inequality is called a cut if it excludes \hat{x}
- Example: $c(x) \leq 0$ convex, and $\exists i : c_i(\hat{x}) > 0$, then

$$0 \geq \hat{c}_i + \nabla \hat{c}^{\mathsf{T}}(x - \hat{x})$$

cuts off \hat{x} . Proof: Exercise.

- Used in Benders decomposition and outer approximation.
- MILP: cuts are basis for branch-and-cut techniques.



Outline



2 Nonlinear Branch-and-Bound







Natural Relaxation (Convex MINLP)

• For a convex MINLP

$$(x_1 - 2)^2 + (x_2 + 1)^2 \le 36$$

 $3x_1 - x_2 \le 6$
 $0 \le x_1, x_2 \le 5$
 $x_2 \in \mathbb{Z}$



Natural Relaxation (Convex MINLP)

• For a convex MINLP

$$(x_1 - 2)^2 + (x_2 + 1)^2 \le 36$$

 $3x_1 - x_2 \le 6$
 $0 \le x_1, x_2 \le 5$
 $x_2 \in \mathbb{R}$

• Dropping integrality results in a convex, nonlinear relaxation



Natural Relaxation (Convex MINLP)

• For a convex MINLP

$$(x_1 - 2)^2 + (x_2 + 1)^2 \le 36$$

 $3x_1 - x_2 \le 6$
 $0 \le x_1, x_2 \le 5$
 $x_2 \in \mathbb{R}$

- Dropping integrality results in a convex, nonlinear relaxation
- Ideal relaxation is convex hull of feasible points
- Optimizing linear function over this convex set solves the problem!



Nonlinear Convex Continuous Relaxation

Relaxing integrality gives convex NLP

```
Nonlinear Relaxation
```

```
\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to } c(x) \leq 0 \\ & x \in \mathcal{X} \\ & x_i \in \mathbb{R} \text{ for all } i \in \mathcal{I} \end{array}
```

```
(NLP_{relax})
```

- Convex optimization problem \Rightarrow unique minimum
- NLP solvers guaranteed to find global minimum

Branching

- Solution x' of (NLP_{relax}) feasible but not integral:
 - Find a nonintegral variable, say $x'_i, i \in I$.
 - Introduce two child nodes with bounds $(I^-, u^-) = (I^+, u^+) = (I, u)$ and setting:

$$u_i^- := \lfloor x_i'
floor, \text{ and } I_i^+ := \lceil x_i'
ceil$$

 \Rightarrow two problems NLP_(l⁻,u⁻), NLP_(l⁺,u⁺) (down/up branch)

Node NLPs

$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to } c(x) \leq 0 \\ & x \in \mathcal{X} \\ & l_i \leq x_i \leq u_i \end{array} \tag{NLP}_{(l,u)})$$

Branching

- Solution x' of (NLP_{relax}) feasible but not integral:
 - Find a nonintegral variable, say $x'_i, i \in I$.
 - Introduce two child nodes with bounds $(I^-, u^-) = (I^+, u^+) = (I, u)$ and setting:

$$u_i^- := \lfloor x_i'
floor$$
, and $l_i^+ := \lceil x_i'
floor$

 \Rightarrow two problems NLP_(I⁻,u⁻), NLP_(I⁺,u⁺) (down/up branch)

Pruning Rules

- (NLP_(I,u)) infeasible \Rightarrow NLPs in subtree also infeasible
- 2 Integer feasible solution $x^{(l,u)}$ of $(NLP_{(l,u)})$:
 - If $f(x^{(l,u)}) < U$, then new $x^* = x^{(l,u)}$ and $U = f^{(l,u)}$.
 - prune node no better solution in subtree
- Solution Optimal value of $(NLP_{(l,u)})$, $f(x^{(l,u)}) \ge U$
 - \Rightarrow prune node: no better integer solution in subtree

Solve relaxed NLP ($0 \le x \le 1$) ... solution gives lower bound

() Solve NLPs & branch on x_i until



Solve relaxed NLP ($0 \le x \le 1$) ... solution gives lower bound

- Solve NLPs & branch on x_i until
- Node infeasible:



Solve relaxed NLP ($0 \le x \le 1$) ... solution gives lower bound

- Solve NLPs & branch on x_i until
- Ø Node infeasible:
- Node integer feasible: ⇒ get upper bound (U)



Solve relaxed NLP ($0 \le x \le 1$) ... solution gives lower bound

- Solve NLPs & branch on x_i until
- 2 Node infeasible:
- Solution Node integer feasible: \Box \Rightarrow get upper bound (U)
- Lower bound $\geq U$:

Search until no unexplored nodes

It Works Theorem

Assume that:

- X bounded polyhedral set;
- NLP solver returns global min.
- \Rightarrow BnB terminates at optimal solution



```
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_{(I,u)}) from heap: \mathcal{H} = \mathcal{H} - \{ NLP_{(I,u)} \}.
    Solve (NLP<sub>(1,u)</sub>) \Rightarrow solution x^{(1,u)}
    if (NLP_{(I,u)}) is infeasible then
         Prune node: infeasible
    else if f(x^{(l,u)}) > U then
         Prune node; dominated by bound U
    else if x_{\tau}^{(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})
    end
end
```

Advanced Nonlinear BnB

Basic BnB will work, but needs improvements:

• Selection of branching variables ... ideally minimize tree to search

... estimate importance of variables from change in objective bounds

- Node selection strategies
 - ... depth-first to find incumbent quickly
- Inexact NLP solves & hot-starts
 ... possible to search tree using QP (or LP solves)
- Cutting planes & branch-and-cut more later
- Software design & modern solvers, e.g. MINOTAUR
- Presolve & reformulations \Rightarrow better models

Presolve for Mixed-Integer Linear Optimization [Savelsbergh, 1994]

Outline

1 Problem Definition and Assumptions

- 2 Nonlinear Branch-and-Bound
- 3 Multi-Tree Methods
- 4 Single-Tree Methods

Motivation MINLP Trees are Huge



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

- Requires solution of thousands of NLPs QP solves can be good alternative
- Can we have even faster solves at nodes? Consider 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 [Duran and Grossmann, 1986]
- Benders decomposition [Geoffrion, 1972]
- Extended cutting plane method [Westerlund and Pettersson, 1995]

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

Multi-tree methods evaluate functions "only" at integer points!

Mixed-Integer Nonlinear Program (MINLP)

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

NLP subproblem for fixed integers $x_{\mathcal{I}}^{(j)}$

$$\mathsf{NLP}(\mathbf{x}_{\mathcal{I}}^{(j)}) \begin{cases} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to } c(x) \leq 0 \\ & x \in \mathcal{X} \quad \text{and } x_{\mathcal{I}} = x_{\mathcal{I}}^{(j)} \end{cases}$$

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

If $(NLP(x_{\mathcal{I}}^{(j)}))$ infeasible then solve feasibility problem ...

,

Mixed-Integer Nonlinear Program (MINLP)

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



 $(F(x_{\mathcal{I}}^{(j)}))$ generalize minimum norm solution ... provides certificate that $(NLP(x_{\mathcal{I}}^{(j)}))$ infeasible





Separate infeasible points by

- Solving NLP for fixed integers to generate cut
- Collect cuts in MILP master problem

Convexity of f and c implies that

Lemma (Supporting Hyperplane)

Linearization about solution $x^{(j)}$ of $(NLP(x_{\mathcal{I}}^{(j)}))$

$$\eta \ge f^{(j)} + \nabla f^{(j)^{T}}(x - x^{(j)})$$

and

$$0 \ge c^{(j)} + \nabla c^{(j)^{T}}(x - x^{(j)}),$$

are outer approximations (OA) of the feasible set of η -MINLP.

Lemma (Feasibility Cuts – Exercise Tomorrow)
If
$$(NLP(x_{\mathcal{I}}^{(j)}))$$
 infeasible, then (OA) cuts off $x_{\mathcal{I}} = x_{\mathcal{I}}^{(j)}$.

Mixed-Integer Nonlinear Program (η -MINLP)

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

Define index set of all possible feasible integers, ${\cal F}$

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

... boundedness of \mathcal{X} implies $|\mathcal{F}| < \infty$ Construct equivalent OA-MILP (outer approximation MILP)

Outer Approximation in Less Than 1000 Words



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

$$U^k := \min_{j \leq k} \left\{ f^{(j)} \mid (\mathsf{NLP}(x_{\mathcal{I}}^{(j)})) \text{ is feasible }
ight\}.$$

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

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

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

Alternate between solve $NLP(y_i)$ and MILP relaxation



$\mathsf{MILP} \Rightarrow \mathsf{lower \ bound}; \qquad \mathsf{NLP} \Rightarrow \mathsf{upper \ bound};$

... convergence follows from convexity & finiteness

Alternate between solve $NLP(y_i)$ and MILP relaxation



 $\mathsf{MILP} \Rightarrow \mathsf{lower \ bound}; \qquad \mathsf{NLP} \Rightarrow \mathsf{upper \ bound};$

... convergence follows from convexity & finiteness

Outer approximation ;

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

repeat

Solve $(NLP(x_{\mathcal{I}}^{(k)}))$ or $(F(x_{\mathcal{I}}^{(k)}))$; solution $x^{(k)}$.; if $(NLP(x_{\mathcal{I}}^{(k)}))$ feasible & $f^{(k)} < U^{k-1}$ then | Update best point: $x^* = x^{(k)}$ and $U^k = f^{(k)}$.; else | Set $U^k = U^{k-1}$.; end Linearize f and c about $x^{(j)}$ and set $\mathcal{F}^k = \mathcal{F}^{k-1} \cup \{k\}$. ; Solve $(M(\mathcal{F}^k))$, let solution be $x^{(k+1)}$ & set k = k + 1. ; until $MILP(M(\mathcal{F}^k))$ is infeasible;

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^(j)_L))
 ⇒ η ≥ f^(j) for feasible point of (M(F^k))
 ... ensures finiteness, since X compact
- Convexity ⇒ linearizations are supporting hyperplanes
 … ensures optimality

Benders Decomposition (Exercise ... add ECP???)

Can derive Benders cut from outer approximation:

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

$$\begin{array}{rcl} \eta \geq & f^{(j)} + \nabla f^{(j)^{T}}(x - x^{(j)}) \\ & + & \lambda^{(j)^{T}} \left(\ 0 \geq & c^{(j)} + \nabla c^{(j)^{T}}(x - x^{(j)}) \ \right) \\ & & \eta \geq & f^{(j)} + \nabla_{\mathcal{I}} \mathcal{L}^{(j)^{T}}(x_{\mathcal{I}} - x_{\mathcal{I}}^{(j)}) \end{array}$$

• 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 $x_{\mathcal{I}}$. Can write cut as $\eta \ge f^{(j)} + \mu^{(j)^{T}}(x_{\mathcal{I}} - x_{\mathcal{I}}^{(j)})$, where $\mu^{(j)}$ multiplier of $x = x_{\mathcal{I}}^{(j)}$ in $(\mathsf{NLP}(x_{\mathcal{I}}^{(j)}))$

Benders Decomposition

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

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

Readily extended to situations where $(NLP(x_{\mathcal{I}}^{(j)}))$ not feasible.

Summary of Multi-Tree Methods

Three Classes of Multi-Tree Methods (did not discuss ECP)

- Outer approximation based on first-order expansion
- Benders decomposition linear combination of OA cuts
- Section 2 Sec

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

1 Problem Definition and Assumptions

- 2 Nonlinear Branch-and-Bound
- 3 Multi-Tree Methods



Aim: avoid solving expensive MILPs

• Start solving master MILP ... using MILP branch-and-cut



Aim: avoid solving expensive MILPs

- Start solving master MILP ... using MILP branch-and-cut
- If x_l^(j) integral, then interrupt MILP; solve NLP(x_l^(j)) get x^(j)



Aim: avoid solving expensive MILPs

- Start solving master MILP ... using MILP branch-and-cut
- If x_l^(j) integral, then interrupt MILP; solve NLP(x_l^(j)) get x^(j)
- Linearize f, c about x^(j)
 ⇒ add linearization to tree



Aim: avoid solving expensive MILPs

- Start solving master MILP ... using MILP branch-and-cut
- If x_l^(j) integral, then interrupt MILP; solve NLP(x_l^(j)) get x^(j)
- Linearize f, c about x^(j)
 ⇒ add linearization to tree
- Continue MILP tree-search



Aim: avoid solving expensive MILPs

- Start solving master MILP ... using MILP branch-and-cut
- If x_l^(j) integral, then interrupt MILP; solve NLP(x_l^(j)) get x^(j)
- Linearize f, c about x^(j)
 ⇒ add linearization to tree
- Continue MILP tree-search
- \dots until lower bound \geq upper bound

Software:

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



$\ensuremath{\mathsf{LP}}\xspace/\ensuremath{\mathsf{NLP}}\xspace$ Branch and Bound

 $\mathsf{LP}/\mathsf{NLP}\text{-}\mathsf{based} \ \mathsf{branch}\text{-}\mathsf{and}\text{-}\mathsf{bound}$

- Branch-and-cut algorithm with cuts from NLP solves
- Create MILP relaxation of MINLP



- Search MILP-tree \Rightarrow faster re-solves
- Interrupt MILP tree-search to create new linearizations

$\ensuremath{\mathsf{LP}}\xspace{\mathsf{NLP}}$ Branch and Bound

LP/NLP-based branch-and-bound

- Branch-and-cut algorithm with cuts from NLP solves
- Create MILP relaxation of MINLP & refine linearizations



- Search MILP-tree \Rightarrow faster re-solves
- Interrupt MILP tree-search to create new linearizations

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.

Abhishek, K., Leyffer, S., and Linderoth, J. T. (2010).

FilMINT: An outer-approximation-based solver for nonlinear mixed integer programs.

INFORMS Journal on Computing, 22:555–567. DOI:10.1287/ijoc.1090.0373.



Bonami, P., Biegler, L., Conn, A., Cornuéjols, G., Grossmann, I., Laird, C., Lee, J., Lodi, A., Margot, F., Sawaya, N., and Wächter, A. (2008). An algorithmic framework for convex mixed integer nonlinear programs. *Discrete Optimization*, 5(2):186–204.



Duran, M. A. and Grossmann, I. (1986).

An outer-approximation algorithm for a class of mixed-integer nonlinear programs.

Mathematical Programming, 36:307-339.



Geoffrion, A. M. (1972).

Generalized Benders decomposition. Journal of Optimization Theory and Applications, 10(4):237–260.



Savelsbergh, M. W. P. (1994).

Preprocessing and probing techniques for mixed integer programming problems. *ORSA Journal on Computing*, 6:445–454.



Westerlund, T. and Pettersson, F. (1995). A cutting plane method for solving convex MINLP problems. *Computers & Chemical Engineering*, 19:s131–s136.