

Mixed-Integer Nonlinear Optimization: Convex MINLPs

GIAN Short Course on Optimization: Applications, Algorithms, and Computation

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Outline









Montivation 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!

Multi-Tree Methods

Recall the $\eta\text{-}\mathsf{MINLP}$ formulation

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

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

Use η -MINLP in this section

Outer Approximation

Mixed-Integer Nonlinear Program (MINLP)

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

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

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

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

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

Outer Approximation

Convexity of f and c implies that

Lemma (Supporting Hyperplane)

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

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

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

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

Outer Approximation

Mixed-Integer Nonlinear Program (η -MINLP)

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

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

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

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

Worst Case Example of Outer Approximation [Hijazi et al., 2010] construct infeasible MINLP:

minimize 0
subject to
$$\sum_{i=1}^{n} \left(y_i - \frac{1}{2}\right)^2 \le \frac{n-1}{4}$$
$$y \in \{0,1\}^n$$

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 2ⁿ vertices

Benders Decomposition

Can derive Benders cut from outer approximation:

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

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

• 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
- Ø 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









Aim: avoid solving expensive MILPs

 Form MILP outer approximation



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- Form MILP outer approximation
- Take initial MILP tree



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



Aim: avoid solving expensive MILPs

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



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 $(x_{l}^{(j)})$ 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.



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

1 Multi-Tree Methods

2 Single-Tree Methods





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



5000+ nodes after solving for 200s

250+ nodes after solving for 45s

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

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

 $0 \le x_1 \le 14$
 $x_2 \in \{0, 1\}$



$$[If x_2 = 1]$$
$$x_1 \le 9$$
(1) is tight.

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

Improving Coefficients: Linear to Nonlinear

Improving Coefficients: Linear to Nonlinear

$$c(x_1, x_2, \dots, x_k) \le M(1 - x_0)$$

 $l_i \le x_i \le u_i, \quad i = 1, \dots, k$
 $x_0 \in \{0, 1\}$

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

Let
$$c^{u} = \max_{x} c(x_1, \dots, x_k)$$
 (MAX-c)
s.t. $l_i \le x_i \le u_i, \quad i = 1, \dots, k$

• If $c^{\boldsymbol{u}} < M$, then tighten: $c(x_1, \ldots, x_k) \leq c^{\boldsymbol{u}}(1-x_0)$

Improving Coefficients: Linear to Nonlinear

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

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- If $c^{\boldsymbol{u}} < M$, then tighten: $c(x_1, \ldots, x_k) \leq c^{\boldsymbol{u}}(1-x_0)$
- (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

$$c(x_1, x_2, \dots, x_k) \leq M(1 - x_0),$$

 $l_i \leq x_i \leq u_i, \quad i = 1, \dots, k,$
 $x_0 \in \{0, 1\}.$

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

$$egin{aligned} c(x_1, x_2, \dots, x_k) &\leq M(1-x_0) \ 0 &\leq x_1 &\leq M_1 x_0 \ 0 &\leq x_2 &\leq M_2 x_0 \end{aligned}$$

. . .

 $x_0\in\{0,1\}$

Improving Coefficients: Using Implications

$$c(x_1, x_2, \dots, x_k) \leq M(1 - x_0),$$

 $l_i \leq x_i \leq u_i, \quad i = 1, \dots, k,$
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• $x_0 = 0 \Rightarrow x_1 = x_2, \ldots = x_k = 0$. (Implications) • If $c(0, \ldots, 0) < M$, then we can tighten. Improving Coefficients: Using Implications

$$c(x_1, x_2, \dots, x_k) \leq M(1 - x_0),$$

 $l_i \leq x_i \leq u_i, \quad i = 1, \dots, k,$
 $x_0 \in \{0, 1\}.$

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

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- $x_0 = 0 \Rightarrow x_1 = x_2, \ldots = x_k = 0$. (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



Full Presolve

Δ

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.

Nonlinear disaggregation [Tawarmalani and Sahinidis, 2005]

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

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

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

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

Lemma

S is projection of S_d onto x.

Consider

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

and

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

Theorem

Any outer approximation of S_d is stronger than OA of S

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

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

$$S^{oa}_{d} := \left\{ (x, y) : h^{(l)} + \nabla h^{(l)^{T}} (y - g(x^{(l)})) \le 0, \\ y \ge g^{(l)} + \nabla g^{(l)^{T}} (x - x^{(l)}), \ \forall x^{(l)} \in \mathcal{X}^{k} \right\},$$

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

[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 $y \in \mathbb{R}^q$

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

can be shown to be tighter

Recall: Worst Case Example of OA

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

minimize 0
subject to
$$\sum_{\substack{i=1\\x \in \{0,1\}^n}}^n \left(x_i - \frac{1}{2}\right)^2 \le \frac{n-1}{4}$$



Уi

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

Disaggregate
$$\sum \left(x_i - \frac{1}{2}\right)^2 \le \frac{n-1}{4}$$
 as $\sum_{i=1}^n y_i \le 0$ and $\left(x_i - \frac{1}{2}\right)^2 \le$

[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 $e = (1, \dots, 1)$
- OA of disaggregated constraint is

$$\sum_{i=1}^{n} y_{i}, \text{ and } x_{i} - \frac{3}{4} \le y_{i}, \text{ and } \frac{1}{4} - x_{i} \le y_{i},$$

• Using $x_i \in \{0, 1\}$ implies $z_i \ge 0$, implies $\sum z_i \ge \frac{n}{4} > \frac{n-1}{4}$ \Rightarrow OA-MILP master of $x^{(1)}$ and $x^{(2)}$ is infeasible. ... terminate in two iterations

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