

ZIB Guest Lecture Mixed-Integer Nonlinear Optimization

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Collaborators







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Outline

1 Problem, Notation, and Definitions

- 2 Modeling in Mixed-Integer Nonlinear Programming
 - Basic Modeling Practice
 - Design of Water Distribution Networks
 - Optimization of IEEE 802.11 Broadband Networks

8 Algorithms for Mixed-Integer Nonlinear Programming

- Basic Building Blocks of MINLP Methods
- Nonlinear Branch and Bound
- Outer Approximation Algorithms
- What Could Go Wrong in MINLP
 - 5 Take-Home Message

Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

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

- $f: \mathbb{R}^n \to \mathbb{R}, \ c: \mathbb{R}^n \to \mathbb{R}^m$ smooth (often convex) functions
- $X \in \mathbb{R}^n$ bounded, polyhedral set, e.g. $X = \{x : l \le A^T x \le u\}$
- $I \subset \{1, \ldots, n\}$ subset of integer variables
- $x_i \in \mathbb{Z}$ for all $i \in I$... combinatorial problem
- Combines challenges of handling nonlinearities with combinatorial explosion of integer variables
- More general constraints possible, e.g. $l \le c(x) \le u$ etc.

Complexity of MINLP

Mixed-Integer Nonlinear Program (MINLP)

```
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```

Complexity of MINLP

- MINLP is NP-hard: includes MILP, which are NP-hard [Kannan and Monma, 1978]
- Worse: MINLP are undecidable [Jeroslow, 1973]: quadratically constrained IP for which no computing device can compute the optimum for all problems in this class ... but we're OK if X is compact!

Convexity of Nonlinear Functions

MINLP techniques distinguish convex and nonconvex MINLPs. For our purposes, we define convexity as ...

Definition

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex, iff $\forall x^{(0)}, x^{(1)} \in \mathbb{R}^n$ we have:

$$f(x^{(1)}) \ge f(x^{(0)}) + (x^{(1)} - x^{(0)})^T \nabla f^{(0)}$$

In a slight abuse of notation, we say that ...

Definition

MINLP is a *convex* if the problem functions f(x) and c(x) are convex functions. If either f(x) or any $c_i(x)$ is a nonconvex function, then MINLP is *nonconvex*.



Convexity (cont.)

We also define the convex hull of a set S as ...

Definition

For a set S, the convex hull of S is conv(S):

$$\left\{x|x=\lambda x^{(1)}+(1-\lambda)x^{(0)}, \ orall 0\leq\lambda\leq 1, \ orall x^{(0)},x^{(1)}\in \mathcal{S}
ight\}.$$

- If $X = \{x \in \mathbb{Z}^p : l \le x \le u\}$ and $l \in \mathbb{Z}^p$, $u \in \mathbb{Z}^p$, then $conv(X) = [l, u]^p$
- Finding convex hull is hard, even for polyhedral X.
- Convex hull important for MILP ...

Theorem

MILP can be solved as LP over the convex hull of feasible set.

$\mathsf{MILP} \neq \mathsf{MINLP}$

Important difference between MINLP and MILP

minimize
$$\sum_{i=1}^{n} (x_i - \frac{1}{2})^2$$
, subject to $x_i \in \{0, 1\}$

... solution is not extreme point (lies in interior) Remedy: Introduce objective η and a constraint $\eta \ge f(x)$

$$egin{aligned} & \min_{\eta,x} & \eta, \ & \text{subject to } f(x) \leq \eta, \ & c(x) \leq 0, \ & x \in X, \ & x_i \in \mathbb{Z}, \ & orall i \in I. \end{aligned}$$

Assume wlog that MINLP objective is linear



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MINLP Modeling Practices

Modeling plays a fundamental role in MILP see [Williams, 1999] ... even more important in MINLP

- MINLP combines integer and nonlinear formulations
- Reformulations of nonlinear relationships can be convex
- Interactions of nonlinear functions and binary variables
- Sometimes we can linearize expressions

MINLP Modeling Preference

We prefer linear over convex over nonconvex formulations.

Convexification of Binary Quadratic Programs

Consider pure binary quadratic function

$$q(x) = x^T Q x + g^T x$$
 where $x \in \{0, 1\}^p$

Let λ be smallest eigenvalue of ${\it Q}$

If $\lambda \geq 0$ then q(x) is convex

Convexification of Binary Quadratics

Let
$$W := Q - \lambda I$$
 and $c := g + \lambda e$, where $e = (1, ..., 1)$,
then $q(x) = x^T W x + c^T x$ is convex.

Linearization of Constraints

Assume $x_2 \neq 0$. A simple transformation (*a* constant parameter):

$$\frac{x_1}{x_2} = a \iff x_1 = ax_2$$

Linearization of bilinear terms x_1x_2 with:

- Binary variable $x_2 \in \{0, 1\}$
- Variable upper bound: $0 \le x_1 \le Ux_2$
- ... introduce new variable x_{12} to replace x_1x_2 and add constraints

$$0 \leq x_{12} \leq x_2 U$$
 and $-U(1-x_2) \leq x_1 - x_{12} \leq U(1-x_2),$

Never Multiply a Nonlinear Function by a Binary

Previous example generalizes to nonlinear functions Often binary variables "switch" constraints on/off

Warning

Never model on/off constraints by multiplying by a binary variable.

Three alternative approaches

- Disjunctive programming, see [Grossmann and Lee, 2003]
- Perspective formulations (not always), see [Günlük and Linderoth, 2012]
- Big-M formulation (weak relaxations)

Goal: Design minimum cost network from discrete pipe diameters to meet water demand





Variables

- q_{ij} : flow pipe $(i,j) \in \mathcal{A}$
- h_i : hydraulic head at node $i \in \mathcal{N}$
- d_{ij} : diameter of pipe $(i, j) \in \mathcal{A}$, where $d_{ij} \in \{P_1, \dots, P_r\}$
- a_{ij} : area of cross section $(i, j) \in \mathcal{A}$
- y_{ijk} : Binary variable = 1 if pipe of size $k \in \mathcal{K}$ chosen for $(i, j) \in \mathcal{A}$

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Constraints

Conservation of flow

$$\sum_{(i,j)\in\mathcal{A}}q_{ij}-\sum_{(j,i)\in\mathcal{A}}q_{ji}=D_i,\ orall i\in\mathcal{N}\setminus\mathcal{S}.$$

• Flow bounds: (linear in *a*, but since $a_{ij} = 0.25\pi d_{ij}^2$, nonlinear in *d*)

$$-V_{\max}a_{ij} \leq q_{ij} \leq V_{\max}a_{ij}, \ orall (i,j) \in \mathcal{A}.$$

- Discrete pipe sizes $d_{ij} \in \{P_1, \ldots, P_r\}$
- Use "multiple choice" integrality to remove nonlinearity $a_{ij} = \pi d_{ij}^2/4$
- This is in general a good modeling practice

- Discrete pipe sizes $d_{ij} \in \{P_1, \ldots, P_r\}$
- Use "multiple choice" integrality to remove nonlinearity $a_{ij} = \pi d_{ij}^2/4$
- This is in general a good modeling practice
- **1** Binary variables $y_{ijk} \in \{0,1\}$ for $k \in \mathcal{K}$
- Ø Model discrete choice as

$$\sum_{k \in \mathcal{K}} y_{ijk} = 1$$
, and $\sum_{k \in \mathcal{K}} P_k y_{ijk} = d_{ij}$. $\forall (i,j) \in \mathcal{A}$

• Model $a_{ij} = \pi d_{ij}^2/4$ (nonlinear) as

$$a_{ij} = \sum_{k \in \mathcal{K}} \left(\frac{\pi}{4} P_k \right)^2 y_{ijk} \; \forall (i,j) \in \mathcal{A}$$

• Nonsmooth, nonlinear pressure loss as a function of flow q_{ij} along arc $(i, j) \in A$ and diameter d_{ij} :

$$h_i - h_j = \kappa_{ij} d_{ij}^{-c_1} \operatorname{sgn}(q_{ij}) |q_{ij}|^{c_2} \quad orall (i,j) \in \mathcal{A}$$

 Nonsmooth, nonlinear pressure loss as a function of flow q_{ij} along arc (i, j) ∈ A and diameter d_{ij}:

$$h_i - h_j = \kappa_{ij} d_{ij}^{-c_1} \operatorname{sgn}(q_{ij}) |q_{ij}|^{c_2} \quad \forall (i,j) \in \mathcal{A}$$

 Another trick: disaggregate flow into flow variables for each pipe size:

$$egin{aligned} q_{ij} &= \sum_{k \in \mathcal{K}} q_{ijk} \ (-V_{\mathsf{max}} a_{ij}) y_{ijk} &\leq q_{ijk} \leq (V_{\mathsf{max}} a_{ij}) y_{ijk} \end{aligned}$$



Why On Earth?

- Doing this allows us to write the (nonlinear) headloss as a function of a single variable q_{ijk}
- Often in applications, the nonlinearity is low-dimensional (low ∈ {1,2})



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Luedtke's Theorem!

Note also that

$$y_{ijk} = 0 \Rightarrow q_{ijk} = 0$$



Optimize 802.11 broadband networks for resource sharing meshes

- objective: minimizing co-channel and inter-channel interference
- integrality: assign channels to basic nodes within a network
- 13 Direct Sequence Spread Spectrum (DSSS) overlapping channels
- co-channel interference: two access points with same channel
- inter-channel interference: cards with overlapping channels transmit simultaneously
- \Rightarrow general nonconvex MINLP

Original model has one horrible constraint ...















• highly nonlinear/nonconvex

•
$$z = 0$$
, if $x \neq y$

- x, y integer (channels)
- model as MIP not NLP





Exercise

Assuming that $0 \le x, y \le U$ are integers, derive an equivalent linear model.

2

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Relaxation and Constraint Enforcement

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_I

Classes of Relaxations for Convex MINLP



Nonlinear and polyhedral relaxation

Solve continuous "natural" NLP relaxations ... branch to "enforce" integrality



... creates branch-and-bound tree

Solve NLP relaxation (x_l continuous, not integer)

minimize f(x) subject to $g(x) \le 0, x \in X$

- 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:

$$\begin{cases} \underset{x}{\text{minimize } f(x),} \\ \text{subject to } g(x) \leq 0, \\ x \in X, \\ l_i \leq x_i \leq u_i, \ \forall i \in I. \end{cases}$$
 (NLP(*I*, *u*))

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

Branching: solution x' of (NLP(I, u)) 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 $l_i^+ := \lceil x_i'
floor$

 $\Rightarrow {\sf create} ~ {\sf NLP}(\mathit{I^-}, \mathit{u^-}) ~/~ {\sf NLP}(\mathit{I^+}, \mathit{u^+}) ~ ({\sf down/up} ~ {\sf branch})$

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Pruning Rules: Let U upper bound on solution

- (NLP(l, 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 $U = f^{(l,u)}$.
 - Otherwise, prune node: no better solution in subtree
- Optimal value of (NLP(I, u)), $f(x^{(I,u)}) \ge U$

 \Rightarrow prune node: no better integer solution in subtree

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

Solve NLPs & branch on x_i until



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

9 Solve NLPs & branch on x_i until

Ode infeasible:



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

- Solve NLPs & branch on x_i until
- Ø Node infeasible:
- Ode 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
- Ode infeasible:
- Solution Node integer feasible: □
 ⇒ get upper bound (U)
- Lower bound $\geq U$:

Search until no unexplored nodes

Theorem (Convergence)

Assume that:

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



BnB trees can get pretty large



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

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

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Common Theme in MINLP

Extend proven MILP techniques to MINLP

Relaxations of Nonlinear Convex Constraints

Relaxing Convex Constraints

Convex 0 ≥ c(x) and η ≥ f(x) 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.



MILP Master Problem & Relaxations

Mixed-Integer Nonlinear Program (MINLP)

 $\underset{x}{\text{minimize } f(x) \text{ subject to } g(x) \leq 0, x \in X, \text{ and } x_i \in \mathbb{Z} \text{ for all } i \in I$

Equivalent MILP master problem for f, g convex:

$$\begin{cases} \underset{\eta,x}{\text{minimize } \eta} \\ \text{subject to } \eta \geq f^{(k)} + \nabla f^{(k)^{T}}(x - x^{(k)}), & \forall k \in \mathcal{K} \\ 0 \geq g^{(k)} + \nabla g^{(k)^{T}}(x - x^{(k)}), & \forall k \in \mathcal{K} \\ x \in X, x_{i} \in \mathbb{Z} \text{ for all } i \in I \end{cases}$$

where
$$\exists$$
 finite set $\mathcal{K} = \left\{ k : x^{(k)} \in X, x_l^{(k)} \in \mathbb{Z}^p \right\}$ and $f^{(k)} = f(x^{(k)})$ etc.

MILP relaxation use $\mathcal{J} \subset \mathcal{K}$

$\ensuremath{\mathsf{LP}}\xspace/\ensuremath{\mathsf{NLP}}\xspace$ 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

$\ensuremath{\mathsf{LP}}\xspace/\ensuremath{\mathsf{NLP}}\xspace$ 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

Aim: avoid perform tree-search on "cheaper" MILP tree NLP subproblem for fixed \hat{x}_{l} :

$$\mathsf{NLP}(\hat{x}_{I}) \begin{cases} \min_{x} f(x) \\ \text{s.t. } g(x) \leq 0, \ x_{I} = \hat{x}_{I} \end{cases}$$

Relax MILP master

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- Relax MILP master
- Start initial MILP tree



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- Relax MILP master
- Start initial MILP tree
- interrupt MILP, when $x_l^{(j)}$ integral
 - solve NLP $(x_l^{(j)})$ get $x^{(j)}$
 - linearize f, c about $x^{(j)}$
 - add linearization to tree



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- continue MILP tree-search
- ... until lower bound \geq upper bound



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- ... until lower bound \geq upper bound



Outer Approximation, Benders Decomposition & ECP Alternate between solve of $NLP(x_I)$ and MILP relaxation



 $\begin{aligned} \text{MILP} \Rightarrow \text{lower bound}; & \text{NLP} \Rightarrow \text{upper bound} \\ \text{Snag: Solve multiple MILPs } ... \text{ no hot-starts} \end{aligned}$

- Outer approximation [Duran and Grossmann, 1986]
- Benders decomposition [Geoffrion, 1972]
- Extended cutting plane [Westerlund and Pettersson, 1995]

Solvers for MINLP

Convex	Nonconvex
α-ECP	<i>α</i> -BB
BONMIN	ANTIGONE
DICOPT	BARON
FilMINT	COCONUT
GUROBI†	COUENNE
KNITRO	CPLEX‡
MILANO	LGO
MINLPBB	LindoGlobal
MINOPT	SCIP
MINOTAUR	
SBB	
Xpress†	
†MIQP	‡MIQP/convex MIQP

Open-source and commercial solvers

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 See solution this afternoon!

A•	4	Å

250+ nodes after solving for 45s

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

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

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



$$\begin{array}{c} \text{If } x_2 = 1 \\ x_1 \leq 9 \\ (1) \text{ is tight.} \end{array}$$





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

Improving Coefficients: Using Implications Common MINLP structure: $x_0 \in \{0, 1\}$, and $x_i \in \mathbb{R}$:

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

Improving Coefficients: Using Implications Common MINLP structure: $x_0 \in \{0, 1\}$, and $x_i \in \mathbb{R}$:

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

• $x_0 = 0 \Rightarrow x_1 = x_2, \ldots = x_k = 0$. (Implications)

• If $c^u := c(0, ..., 0) < M$, then we can improve coefficients

$$c(x_1,\ldots,x_k) \leq c^u(1-x_0)$$

harder without $0 \le x_i \le M_i x_0$ (need global minimization)

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



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.

Take Home Messages

- Modeling is extremely important for MINLP
 ... strong relaxations are key
- Effective MILP techniques useful for MINLP ... more work can be done!
- MINLP software maturing,
 - ... but lags behind commercial MILP software
- Linear better than convex better than nonconvex
- Exploit structure whenever possible

MINOTAUR's Soft-Wear Stack



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

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