Modeling with Mixed-Integer Nonlinear Optimization

Summer School on Optimization of Dynamical Systems

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Argonne National Laboratory

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Course Outline: Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Programming (MINLP)

1. Monday, September 3: Two-Part Lecture
   1. Modeling with Mixed-Integer Nonlinear Optimization
   2. Methods for Convex Mixed-Integer Nonlinear Optimization
2. Tuesday, September 4: Two-Part Lecture & Tutorial
   1. Advanced Methods for Convex MINLPs
   2. Methods for Nonconvex Mixed-Integer Nonlinear Optimization
3. Tutorial: 10:30am – Noon (starting with short intro)

Time permitting: Short transition to dynamical MINLPs ...

Outline: Modeling with Mixed-Integer Nonlinear Optimization

1. Problem Definition and Assumptions
2. MINLP Modeling Practices
3. A Short Introduction to AMPL
4. Model: Quadratic Uncapacitated Facility Location

Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

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

- $\mathcal{X}$ bounded polyhedral set, e.g. $\mathcal{X} = \{x \ : \ l \leq A^T x \leq u\}$
- $f : \mathbb{R}^n \to R$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ twice continuously differentiable (sometimes convex)
- $\mathcal{I} \subset \{1, \ldots, n\}$ subset of integer variables
- Relaxations satisfy a constraint qualification (technical)

NP-Super Hard

Challenges of MINLP

Combines challenges of handling nonlinearities
with combinatorial explosion of integer variables

NP-Super Hard

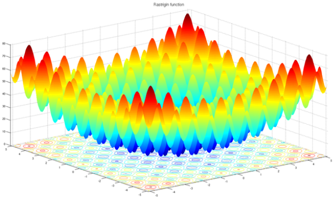
Challenges of MINLP

Combines challenges of handling nonlinearities with combinatorial explosion of integer variables

The great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.
- R. Tyrrell Rockafellar

- If f and c are convex functions, then we have a convex MINLP
- If f and c are not convex, then we have a nonconvex MINLP

The Importance of Being Convex



2D Rastrigin Test Function

Not All Solvers Are Equal

Without convexity, many solvers only guarantee local optimality

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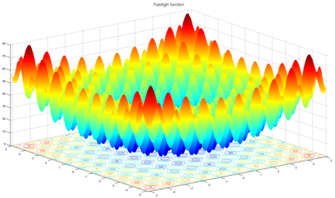

2D Rastrigin Test Function

Not All Solvers Are Equal

Without convexity, many solvers only guarantee local optimality

Impact of Convexity

- Nonconvex MINLPs are much harder to solve
- May not be able to "prove" global optimality
- Make sure you really need nonconvexity in your MINLP!

Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

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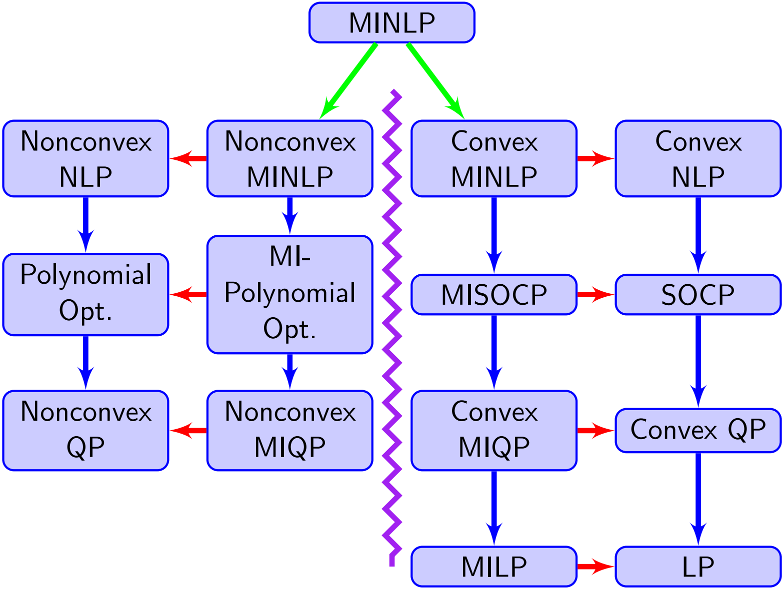
- MINLPs are NP-hard ... includes MILP, which are NP-hard, see [Kannan and Monma, 1978]
- Worse: MINLP are undecidable, see [Jeroslow, 1973]:
  $\exists$ quadratically constrained IP for which no computing device can compute the optimum for all problems in this class
  ... but we're OK if $\mathcal{X}$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

MINLP Specializations

- MISOCP: Mixed Integer Second Order Cone Program
  - Convex-MINLP with $c_i(x) = \|A_i x + b_i\|_2 - p_i^T x + q_i$
- MIPP: Mixed Integer Polynomial Program: $c_i(x)$ polynomial
- MIQP: Mixed Integer Quadratic Program
  - May be convex or nonconvex: $c_i(x) = x^T Q_i x + p_i^T + q_i$
  - Convex MIQP is a special case of MISOCP, if $Q_i \succeq 0$
  - If f is convex quadratic and c is an affine mapping, then there are specialized algorithms for convex-MIQP
- MILP: Mixed Integer Linear Program
  - Most efficient solvers: $c_i(x) = a_i^T x - b_i$

MINLP Tree



MINLP
Nonconvex NLP
Nonconvex MINLP
Convex MINLP
Convex NLP
Polynomial Opt.
MI-Polynomial Opt.
MISOCP
SOCP
Nonconvex QP
Nonconvex MIQP
Convex MIQP
Convex QP
MILP
LP

Practical Complexity $\simeq$ Is There Hope to Solve it?

The Leyffer-Linderoth-Luedtke (LLL) Measure of Complexity

Given a problem of class X with Y decision variables, what is the largest value of Y for which Jim, Jeff, or Sven would be willing to bet \$50 that a "state-of-the-art" solver could solve the problem?

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Convex		Nonconvex	
Problem Class (X)	**# Var** (Y)	**Problem Class** (X)	**# Var** (Y)
MINLP	500	MINLP	100
NLP	5×10^4	NLP	100
MISOCP	1000	MIPP	150
SOCP	10^5	PP	150
MIQP	1000	MIQP	300
QP	5×10^5	QP	300
MILP	2×10^4		
LP	5×10^7		

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1 Problem Definition and Assumptions

2 MINLP Modeling Practices

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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.

Modeling with Integer Variables

Linderoth "Fundamental Theorem of Integer Variables"

97.238% of MINLPs have integer variables for two purposes only:

1. Binary variables to make a "multiple choice" selection
2. Binary indicator variables that turn on/off continuous variables and/or constraints.

1. Multiple Choice Selection

$$y \in \{D_1, D_2, \ldots, D_k\}$$

where D_i are discrete parameters (e.g. pipe diameters)

2. Indicator Variables

$$\text{if } y_i = 1 \text{ then } c_i(x) \leq 0, \quad \text{otherwise } c_i(x) \leq \infty$$

Modeling Multiple Choice Selection

Discrete Choices

We can model $y \in \{D_1, D_2, \ldots, D_k\}$, where D_i discrete parameters as special ordered set (SOS) [Beale and Tomlin, 1970]

$$y = \sum_{i=1}^{k} z_i D_i, \quad 1 = \sum_{i=1}^{k} z_i, \quad z_i \in \{0, 1\}$$

- Similarly linearize univariate functions $f(z)$, $z \in \mathbb{Z}$
- Generalizes to higher dimensions, [Beale and Forrest, 1976]
- Solvers detect SOS structure and use special branching rules

Calculus of Logical Modeling: Indicator/Lookout Variables

1. Indicator variable: $y_i \in \{0,1\}$ to force a constraint to hold

$$y_i = 1 \quad \Rightarrow \quad c_i(x) \le 0$$

can be modeled as

$$y_i \in \{0,1\} \quad \text{and} \quad c_i(x) \le M(1 - y_i)$$

where $M > 0$ is known upper bound on $c(x)$ for $x \in \mathcal{X}$

2. Lookout variable: $y_i \in \{0,1\}$ is forced if a constraint holds

$$a_i^T x + b_i \le 0 \quad \Rightarrow \quad y_i = 1$$

can be modeled as

$$y_i \in \{0,1\} \quad \text{and} \quad a_i^T x + b_i \ge (m - \epsilon) y_i$$

where $m > 0$ lower bound on $a_i^T x + b_i$ for $x \in \mathcal{X}$, and $\epsilon > 0$ ... is tolerance tol (e.g. 10^{-4})

Some Useful Nonlinear Variable Transformations

Design of multiproduct batch plant includes nonconvex terms

$$\sum_{j \in M} \alpha_j N_j V_j^{\beta_j}; \qquad C_i N_j \geq \tau_{ij}; \qquad \sum_{i \in N} \frac{\psi_i}{B_i} C_i \leq \gamma$$

where variables are upper case, parameters are Greek letters.

Introduce log-transform variables:

$$v_j = \ln(V_j), \quad n_j = \ln(N_j), \quad b_i = \ln(B_i), \quad c_i = \ln(C_i)$$

Transformed expressions are convex:

$$\sum_{j \in M} \alpha_j e^{n_j + \beta_j v_j}, \qquad c_i + n_j \geq \ln(\tau_{ij}), \qquad \sum_{i \in N} \psi_i e^{c_i - b_i} \leq \gamma$$

Linearization of Constraints

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

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

Linearization of bilinear terms $x_1 x_2$ with:

- Binary indicator variable $x_2 \in \{0, 1\}$
- Variable upper bound: $0 \leq x_1 \leq U x_2$

... new variable x_{12} replaces $x_1 x_2$ ... using constraints

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

Proof: $x_{12} \in \{0, x_1\}$ follows from constraints.

Never Multiply a Nonlinear Function by a Binary

Previous example generalizes to nonlinear functions: $x_2 c(x_1) \leq 0$

Warning

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

Three alternative approaches

- Disjunctive programming, [Grossmann and Lee, 2003]
- Perspective formulations, [Günlük and Linderoth, 2012]
- Big-M formulation (weak relaxations)

Another Example of Bad Nonlinear Models

Warning

Never replace a binary variable by a nonlinear expression!

We can write a binary constraint, $x \in \{0, 1\}$, equivalently as

$$0 \leq x \leq 1 \quad \text{and} \quad x(1-x) = 0$$

or also as a complementarity constraint ...

$$0 \leq x \ \perp x \leq 1$$

... both are bad ... hide integrality from solvers!

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A Short Introduction to AMPL

AMPL: A Mathematical Programming Language

- Algebraic modeling language for optimization
- Three main model/instance components
  1. Model file (describes algebraic form of equations) `*.mod`
  2. Data file (describe data of the instance) `*.dat`
  3. Command file (optional: describe control sequence) `*.ampl`
- Link to solvers (binaries compiled with AMPL-solver interface)

  1. NLP Solvers: CONOPT, Knitro, LOQO, Minos, SNOPT
  2. MINLP Solvers: Baron, KNITRO
  3. MILP Solvers: GuRoBi, XPRESS

Other AMPL Solvers

- Minotaur (Argonne) download and binaries (Linux/MacOS) https://wiki.mcs.anl.gov/minotaur/index.php/Minotaur_Download
- COIN-OR Project https://www.coin-or.org/projects/

Collections of MINLP Test Problems

AMPL Collections of MINLP Test Problems

1. MacMINLP www.mcs.anl.gov/~leyffer/macminlp/
2. IBM/CMU collection egon.cheme.cmu.edu/ibm/page.htm

GAMS Collections of MINLP Test Problems

1. GAMS MINLP-world www.gamsworld.org/minlp/
2. MINLP CyberInfrastructure www.minlp.org/index.php

Solve MINLPs online on the NEOS server,
www.neos-server.org/neos/

... and there are even a few CUTEr problems in SIF!

Introduction to AMPL Modeling Language

We have a full (temporary) license of AMPL for the course

Optimization Problem

$$\min_x \exp(-x_1) + \sum_{i=2}^{3} x_i^2$$

$$\text{s.t. } x_1 \log(x_2) + x_2^3 \geq 1$$

$$5 \geq x_1, x_2, x_3 \geq 0$$

AMPL Formulation

```
var x{1..3} >=0, <=5; # ... variables

minimize              # ... objective functn
 f: exp(-x[1]) + sum{i in 2..3} x[i]^2;

subject to            # ... constraints
 con: x[1]*log(x[2]) + x[2]^3 >= 1;
```

Beware: $x_2 > 0$ ... $\log(x_2)$ undefined for $x_2 \leq 0$!

Running & Trouble Shooting an AMPL Model

1. Create a `*.mod` model file (see file)
2. Start `ampl`; load model (e.g. `simple.mod`); select solver:

```
ampl: reset; model simple.mod;
ampl: option solver ipopt;
ampl: solve;
```

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3. Display the answer or trouble shoot

```
ampl: display _varname, _var.lb, _var, _var.ub;
ampl: display _conname, _con.lb, _con.body, _con.ub;
ampl: expand;
```

... list variable/constraint name, lower bnd, body, upper bnd
... shows all constraints and objective functions

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   ... list variable/constraint name, lower bnd, body, upper bnd
   ... shows all constraints and objective functions

4. We forgot to ensure $x_2 > 0$ so that $\log(x_2)$ defined:

```
ampl: let x[2] := 1;
ampl: solve;
```

   ... assigns an initial value to x_2 (different from default, 0).

Short Quiz (see `geartrain.mod` in MacMINLP)

Consider the gear-train design problem for best matching gear ratio

$$\underset{x}{\text{minimize}} \quad \left(\frac{1}{6.931} - \frac{x_3 x_2}{x_1 x_4} \right)^2 \qquad x \in \mathbb{Z}^4, \; 12 \le x_i \le 60$$

- Is the problem a convex or nonconvex MINLP?
- Is there an equivalent but simpler formulation?

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Uncapacitated Facility Location

Problem introduced by Günlük, Lee, and Weismantel ('07) and classes of strong cutting planes derived

- M: Facility
- N: Customer
- x_{ij}: percentage of customer $j \in N$ demand met by facility $i \in M$
- $z_i = 1 \Leftrightarrow$ facility $i \in M$ is built
- Fixed cost for opening facility $i \in M$
- Quadratic cost for meeting demand $j \in N$ from facility $i \in M$

Quadratic Uncapacitated Facility Location Problem

- A very simple MIQP

$$z^* \stackrel{\text{def}}{=} \min \sum_{i \in M} c_i z_i + \sum_{i \in M} \sum_{j \in N} q_{ij} x_{ij}^2$$

subject to

$$\begin{aligned} x_{ij} &\leq z_i && \forall i \in M, \forall j \in N \\ \sum_{i \in M} x_{ij} &= 1 && \forall j \in N \\ x_{ij} &\geq 0 && \forall i \in M, \forall j \in N \\ z_i &\in \{0, 1\} && \forall i \in M \end{aligned}$$

Partial AMPL Model for Quadratic facility Location

- Declare variables

```
var x{I,J} >= 0, <= 1; # ... % of customer i served by  j
var z{I} binary;       # ... z_i=1, iff facility i built
```

- Declare objective function

```
minimize quadCost: sum{i in I} C[i]*z[i]
                 + sum{i in I, j in J} Q[i,j]*x[i,j]^2;
```

- Declare constraints

```
subject to

  # ... only serve customers from open facilities
  varUBD{i in I, j in J}: x[i,j] <= z[i];

  # ... meet all customer's demands
  meetDemand{j in J}: sum{i in I} x[i,j] = 1;
```

Missing: Definition of sets `I`,`j`, and data `Q`, `C`!

Base Case of Induction to "Linderoth Theorem"

- Binary variables used as indicators: $z_i = 0 \Rightarrow x_{ij} = 0$
- If $z = 1$, then we need to model the epigraph of x_{ij}^2

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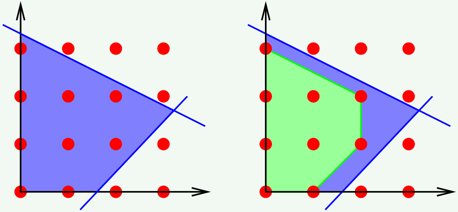
Building on Years of MIP Expertise

- Mixed Integer Linear Programmers carefully study simple problem structures for "good" formulations of problems
- Goal: closely approximate convex hull of feasible points

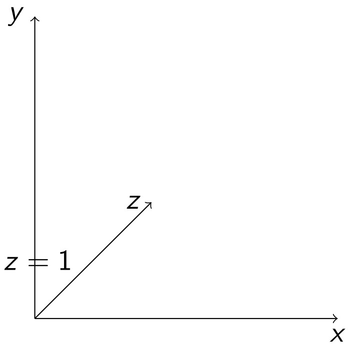


... solve LP relaxation

- Study structure of a special MINLP with indicator variables

A Very Simple Structure

$$R \stackrel{\text{def}}{=} \left\{(x, y, z) \in \mathbb{R}^2 \times \mathbb{B} \mid y \geq x^2, 0 \leq x \leq uz\right\}$$



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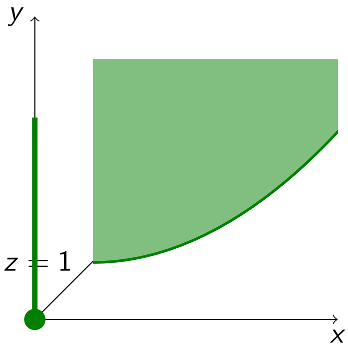
- $z = 1 \Rightarrow x \leq u, y \geq x^2$



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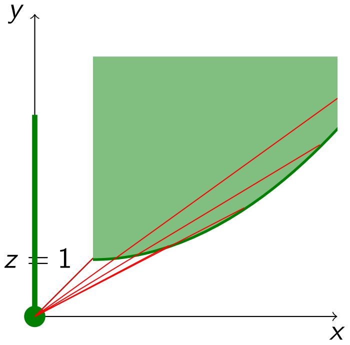

Deep Insights

- $\text{conv}(R) \equiv$ line connecting $\mathbf{0}$ to $y = x^2$ in the $z = 1$ plane

Characterization of Convex Hull

Deep Theorem #1

$$R = \left\{(x, y, z) \in \mathbb{R}^2 \times \mathbb{B} \mid y \geq x^2, 0 \leq x \leq uz\right\}$$

$$\text{conv}(R) = \left\{(x, y, z) \in \mathbb{R}^3 \mid yz \geq x^2, 0 \leq x \leq uz, 0 \leq z \leq 1, y \geq 0\right\}$$

Characterization of Convex Hull

Deep Theorem #1

$$R = \left\{(x,y,z) \in \mathbb{R}^2 \times \mathbb{B} \mid y \geq x^2, 0 \leq x \leq uz\right\}$$

$$\text{conv}(R) = \{(x,y,z) \in \mathbb{R}^3 \mid yz \geq x^2, 0 \leq x \leq uz, 0 \leq z \leq 1, y \geq 0\}$$

$x^2 \leq yz, \quad y, z \geq 0 \equiv$

Second Order Cone Programming

- $\exists$ effective, robust algorithms for optimizing over conv(R)

The Beauty of Cones

Remarkable Result for Convex MINLPs

All 333 convex problems in MINLPLIB2 can be represented with only four types of cones (for $x \in \mathbb{R}^n$) [Lubin et al., 2016]

1. Quadratic cones: $\|x\|_2^2 \le x_0, \quad$ for $x \in \mathbb{R}^n$
2. Rotated quadratic cones: $2x_1x_2 \ge \left(x_3^2 + \ldots + x_n^2\right)^{1/2}$
3. Power cones: $|x|^p \le x_0$ ... or ℓ_p-norms $\|x\|_p \le x_0$
4. Exponential cones: e.g. $e^x \le x_0$

Advantages of Cones

- Convex cones give strong relaxations (more later)
- Build on "Disciplined Convex Modeling" [Grant et al., 2006] to assure convexity

Snag: Need interior-point solvers ... or use cutting planes!

Teaching Points: Modeling MINLPs

Modeling MINLP

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

- Most binary variables used as indicator or lookout variables
- Reformulation tricks are important ... linearization of $x_1 x_2$ for $x_2 \in \{0, 1\}$
- AMPL modeling language: convenient & intuitive

Tighter relaxations/formulations from Conic Programming

- Use of perspective and conic formulations important

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