Topic 6:
Mixed-Integer Nonlinear Optimization

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CENG60008 – Process Optimisation
CENG70003 – Advanced Process Optimisation

Mixed-Integer Nonlinear Programming (MINLP)

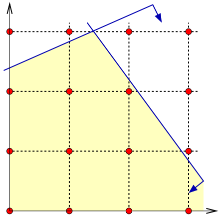
$$\min_{\mathbf{x},\mathbf{y}} \; f(\mathbf{x},\mathbf{y}) \qquad \longleftarrow \quad \text{objective function}$$

$$\text{s.t.} \quad \mathbf{g}(\mathbf{x},\mathbf{y}) \leq \mathbf{0} \qquad \longleftarrow \quad \text{inequality constraints}$$

$$\left.\begin{aligned} &\mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x} \\ &\mathbf{y} \in \{0,1\}^{n_y} \end{aligned}\right. \qquad \longleftarrow \quad \text{variable domain}$$

- f and $\mathbf{g}$ may not be linear or even convex functions

- That optimization problems with binary/integer variables are more difficult to solve than continuous problems may appear counter-intuitive
- The feasible set is nonconnected and therefore inherently nonconvex



MINLP Solution Paradigm

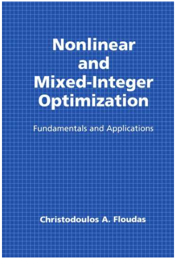
Construct a sequence of related but simpler subproblems that converges (finitely) to the exact MINLP solution

- Use linearization / relaxation to construct the subproblems
  - Both the objective function and the feasible region
- The subproblems should yield valid bounds on the original MINLP
  - Lower bound for a minimize problem
  - Upper bound for a maximize problem
- The subproblems should be easier to solve than the original MINLP
  - Many subproblems may need to be solved!
- The number of subproblems solved should be much smaller than with the complete enumeration method
  - although pathological problems can always be constructed...

Contents

Solving MINLP models is challenging – We will learn some typical decomposition techniques for MINLPs with either convex or nonconvex participating functions

1. Methods for MINLP with Convex Functions
   - Branch-and-Bound Algorithm
   - Outer-Approximation Algorithm
2. Methods for MINLP with Nonconvex Functions



Recommended Readings:

- C.A. Floudas, *Nonlinear and Mixed- Integer Optimization*, Oxford University Press, 1995
- I.E. Grossmann, Review of nonlinear mixed-integer and disjunctive programming techniques, *Optimization & Engineering* **1**:227-252, 2002

Methods for MINLP with Convex Functions

Main Solution Algorithms

$$\begin{aligned}
\min_{\mathbf{x},\mathbf{y}} \;& f(\mathbf{x},\mathbf{y})\\
\text{s.t.}\;& \mathbf{g}(\mathbf{x},\mathbf{y}) \leq \mathbf{0}\\
& \mathbf{x} \in [\mathbf{x}^{\mathrm{L}},\mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x}\\
& \mathbf{y} \in \{0,1\}^{n_y}
\end{aligned}$$

- f and $\mathbf{g}$ are nonlinear and convex functions

- Branch-and-Bound (BB)
  - Ravindran & Gupta (1985); Stubbs & Mehrotra (1999)
- Generalized Benders Decomposition (GBD)
  - Geoffrion (1972)
- Outer Approximation (OA)
  - Duran & Grossmann (1986); Fletcher & Leyffer (1994)
- Extended Cutting Plane (ECP)
  - Westerlund & Pettersson (1995)

Methods for MINLP with Convex Functions

Branch-and-Bound Algorithm

$$\begin{aligned}\min_{\mathbf{x},\mathbf{y}}\ & f(\mathbf{x},\mathbf{y})\\ \text{s.t.}\ & \mathbf{g}(\mathbf{x},\mathbf{y}) \leq \mathbf{0}\\ & \mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x}\\ & \mathbf{y} \in \{0,1\}^{n_y}\end{aligned} \quad \xrightarrow{\text{NLP relax}} \quad \begin{aligned}\min_{\mathbf{x},\mathbf{y}}\ & f(\mathbf{x},\mathbf{y})\\ \text{s.t.}\ & \mathbf{g}(\mathbf{x},\mathbf{y}) \leq \mathbf{0}\\ & \mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x}\\ & \mathbf{y} \in [0,1]^{n_y}\end{aligned}$$

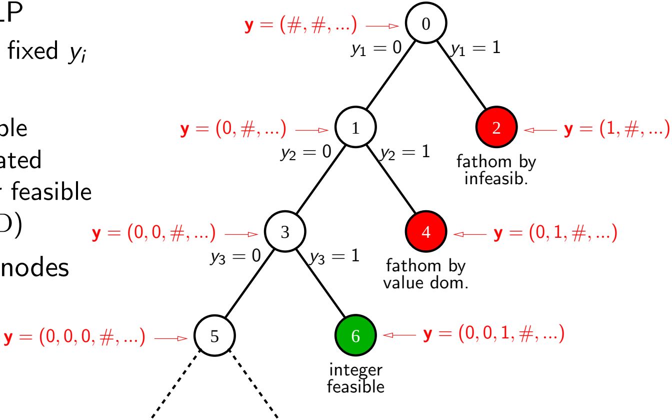
Key Properties:

- If an NLP relaxation is infeasible, so is the MINLP it relaxes
  - But an infeasible MINLP could have a feasible NLP relaxation
- The optimal solution value of an NLP relaxation yields a lower bound on the MINLP it relaxes (minimize case)
- If the optimal solution to an NLP relaxation is integer feasible, it is also optimal for the MINLP it relaxes

Methods for MINLP with Convex Functions

Branch-and-Bound Algorithm

- Branch on fractional y_i
- Solve relaxed NLP
  - Mixed free / fixed y_i
- Fathom if:
  1. Node infeasible
  2. Node dominated
  3. Node integer feasible (update UBD)
- Stop if no open nodes



Convexity is Critical!

Methods for MINLP with Convex Functions

Branch-and-Bound Example

Workshop. Consider the following MINLP model and derive the relaxed NLP model at the root node.

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3 \\
\text{s.t. }\ & (x_1-2)^2 - x_2 \le 0 \\
& x_1 \ge 2y_1 \\
& x_1 - x_2 \le 4(1-y_2) \\
& x_1 \ge (1-y_1) \\
& x_2 \ge y_2 \\
& x_1 + x_2 \ge 3y_3 \\
& y_1 + y_2 + y_3 \ge 1 \\
& 0 \le x_1, x_2 \le 4 \\
& y_1, y_2, y_3 \in \{0,1\}
\end{aligned}
$$

$$\xrightarrow{\text{NLP relax}}$$

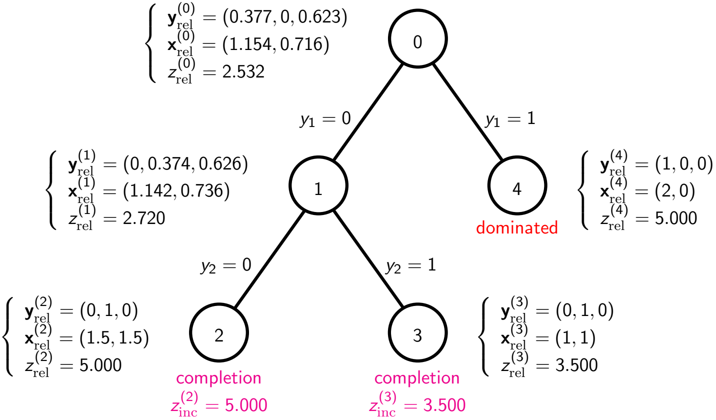
$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3 \\
\text{s.t. }\ & (x_1-2)^2 - x_2 \le 0 \\
& x_1 \ge 2y_1 \\
& x_1 - x_2 \le 4(1-y_2) \\
& x_1 \ge (1-y_1) \\
& x_2 \ge y_2 \\
& x_1 + x_2 \ge 3y_3 \\
& y_1 + y_2 + y_3 \ge 1 \\
& 0 \le x_1, x_2 \le 4 \\
& 0 \le y_1, y_2, y_3 \le 1
\end{aligned}
$$

- Optimal solution: $f^* = 3.5$, $x_1^* = x_2^* = 1$, $y_2^* = 1$, $y_1^* = y_3^* = 0$
- Lower Bound: $\mathrm{LBD}^0 \approx 2.532$, $x_1^0 \approx 1.154$, $x_2^0 \approx 0.716$, $y_1^0 \approx 0.377$, $y_2^0 = 0$, $y_3^0 \approx 0.623$

Methods for MINLP with Convex Functions

Branch-and-Bound Example

Workshop. Apply the branch-and-bound algorithm to the MINLP model, using GAMS to solve the relaxed NLP models – Branch on fractional variables and apply depth-first search.



Methods for MINLP with Convex Functions

Outer-Approximation Algorithm

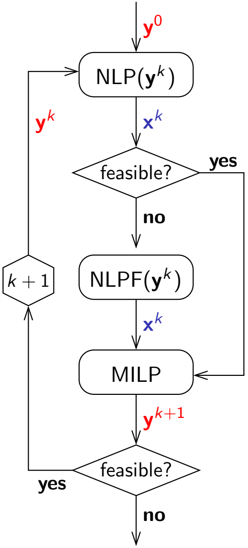
- **Idea.** Alternate solution between NLP and MILP

Primal problem NLP($\mathbf{y}^k$): set $\mathbf{y} = \mathbf{y}^k$ in f and $\mathbf{g}$

$$\begin{aligned} \mathbf{x}^k \in \arg\min_{\mathbf{x}} \ & f(\mathbf{x}, \mathbf{y}^k) \\ \text{s.t. } & \mathbf{g}(\mathbf{x}, \mathbf{y}^k) \leq \mathbf{0} \\ & \mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x} \end{aligned}$$

Primal problem NLPF($\mathbf{y}^k$): if infeasible NLP($\mathbf{y}^k$)

$$\begin{aligned} \mathbf{x}^k \in \arg\min_{\mathbf{x},\omega} \ & \omega \\ \text{s.t. } & \mathbf{g}(\mathbf{x}, \mathbf{y}^k) \leq \omega \\ & \mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x}, \ \omega \geq 0 \end{aligned}$$



Methods for MINLP with Convex Functions

Outer-Approximation Algorithm

- **Idea.** Alternate solution between NLP and MILP

Master problem MILP: linearize f and $\mathbf{g}$ @$(\mathbf{x}^k, \mathbf{y}^k)$

$$\mathbf{y}^{k+1} \in \arg\min_{\mathbf{x},\mathbf{y},\eta} \eta$$

$$\text{s.t. } \forall j \leq k, \text{ feasible NLP}(\mathbf{y}^j):$$

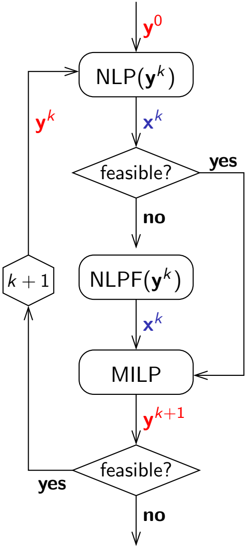
$$f(\mathbf{x}^j, \mathbf{y}^j) + \nabla f(\mathbf{x}^j, \mathbf{y}^j) \begin{bmatrix} \mathbf{x} - \mathbf{x}^j \\ \mathbf{y} - \mathbf{y}^j \end{bmatrix} \leq \eta$$

$$\forall j \leq k:$$

$$\mathbf{g}(\mathbf{x}^j, \mathbf{y}^j) + \nabla \mathbf{g}(\mathbf{x}^j, \mathbf{y}^j) \begin{bmatrix} \mathbf{x} - \mathbf{x}^j \\ \mathbf{y} - \mathbf{y}^j \end{bmatrix} \leq \mathbf{0}$$

$$\mathbf{x} \in [\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}] \subset \mathbb{R}^{n_x}, \ \mathbf{y} \in \{0,1\}^{n_y}$$

- New cuts appended at each iteration: non-decreasing lower bound

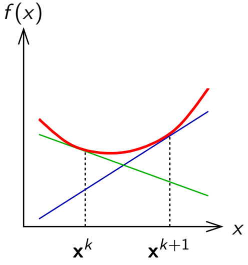


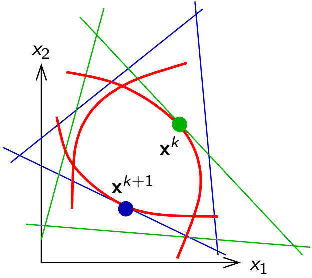
Methods for MINLP with Convex Functions

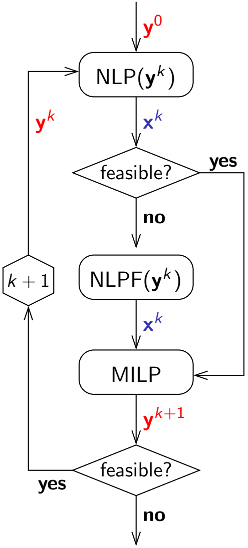
Outer-Approximation Algorithm

- **Idea.** Alternate solution between NLP and MILP

Convexity is Critical!







- **OA Convergence and Performance**
  - Finite termination
  - Fewer NLP subproblems than B&B is typical
  - Solving master MILP can be the bottleneck

Methods for MINLP with Convex Functions

Outer-Approximation Example

Workshop. Consider the following MINLP model and apply the OA algorithm, starting from $\mathbf{y}^0 = (1, 0, 0)$.

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3 \\
\text{s.t. } & (x_1 - 2)^2 - x_2 \leq 0 \\
& x_1 \geq 2y_1 \\
& x_1 - x_2 \leq 4(1 - y_2) \\
& x_1 \geq (1 - y_1) \\
& x_2 \geq y_2 \\
& x_1 + x_2 \geq 3y_3 \\
& y_1 + y_2 + y_3 \geq 1 \\
& 0 \leq x_1, x_2 \leq 4 \\
& y_1, y_2, y_3 \in \{0, 1\}
\end{aligned}
$$

$$\xrightarrow{\text{NLP}(\mathbf{y}^0)}$$

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3 \\
\text{s.t. } & (x_1 - 2)^2 - x_2 \leq 0 \\
& x_1 \geq 2y_1 \\
& x_1 - x_2 \leq 4(1 - y_2) \\
& x_1 \geq (1 - y_1) \\
& x_2 \geq y_2 \\
& x_1 + x_2 \geq 3y_3 \\
& y_1 + y_2 + y_3 \geq 1 \\
& 0 \leq x_1, x_2 \leq 4 \\
& (y_1, y_2, y_3) = (1, 0, 0)
\end{aligned}
$$

➥ Optimal solution: $f^* = 3.5$,
$x_1^* = x_2^* = 1$,
$y_1^* = 0,\ y_2^* = 1,\ y_3^* = 0$

➥ Upper Bound: $\mathrm{UBD}^0 = 5$,
$x_1^0 = 2,\ x_2^0 = 0$,
$y_1^0 = 1,\ y_2^0 = 0,\ y_3^0 = 0$

Methods for MINLP with Convex Functions

Outer-Approximation Example

$\xrightarrow{\text{MILP}}$

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y},\eta}\ & \eta \\
\text{s.t. } & 4x_1 + y_1 + 1.5y_2 + 0.5y_3 - 4 \le \eta \\
& -x_2 \le 0 \\
& x_1 \ge 2y_1 \\
& x_1 - x_2 \le 4(1-y_2) \\
& x_1 \ge (1-y_1) \\
& x_2 \ge y_2 \\
& x_1 + x_2 \ge 3y_3 \\
& y_1 + y_2 + y_3 \ge 1 \\
& 0 \le x_1, x_2 \le 4 \\
& y_1, y_2, y_3 \in \{0,1\}
\end{aligned}
$$

➥ Lower Bound: $\mathrm{LBD}^1 = 0.5$, $x_1^1 = 1,\ x_2^1 = 4,\ y_1^1 = 0,\ y_2^1 = 0,\ y_3^1 = 1$

$\xrightarrow{\text{NLP}(\mathbf{y}^1)}$

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3 \\
\text{s.t. } & (x_1-2)^2 - x_2 \le 0 \\
& x_1 \ge 2y_1 \\
& x_1 - x_2 \le 4(1-y_2) \\
& x_1 \ge (1-y_1) \\
& x_2 \ge y_2 \\
& x_1 + x_2 \ge 3y_3 \\
& y_1 + y_2 + y_3 \ge 1 \\
& 0 \le x_1, x_2 \le 4 \\
& (y_1, y_2, y_3) = (0,0,1)
\end{aligned}
$$

➥ Upper Bound: $\mathrm{UBD}^1 = 5$, $x_1^1 = 1.5,\ x_2^1 = 1.5$, $y_1^1 = 0,\ y_2^1 = 0,\ y_3^1 = 1$

Methods for MINLP with Convex Functions

Outer-Approximation Example

$$\xrightarrow{\text{MILP}}\quad \begin{aligned}\min_{\mathbf{x},\mathbf{y},\eta}\ & \eta\\ \text{s.t.}\ & 4x_1 + y_1 + 1.5y_2 + 0.5y_3 - 4 \le \eta\\ & 3x_1 + 3x_2 + y_1 + 1.5y_2 + 0.5y_3 - 4.5 \le \eta\\ & -x_2 \le 0\\ & -x_1 - x_2 + 1.75 \le 0\\ & x_1 \ge 2y_1\\ & x_1 - x_2 \le 4(1-y_2)\\ & x_1 \ge (1-y_1)\\ & x_2 \ge y_2\\ & x_1 + x_2 \ge 3y_3\\ & y_1 + y_2 + y_3 \ge 1\\ & 0 \le x_1, x_2 \le 4\\ & y_1, y_2, y_3 \in \{0,1\}\end{aligned}$$

➥ Lower Bound: $\mathrm{LBD}^2 = 3$, $x_1^2 = 1,\ x_2^2 = 1,\ y_1^2 = 0,\ y_2^2 = 1,\ y_3^2 = 0$

$$\xrightarrow{\text{NLP}(\mathbf{y}^2)}\quad \begin{aligned}\min_{\mathbf{x},\mathbf{y}}\ & x_1^2 + x_2^2 + y_1 + 1.5y_2 + 0.5y_3\\ \text{s.t.}\ & (x_1-2)^2 - x_2 \le 0\\ & x_1 \ge 2y_1\\ & x_1 - x_2 \le 4(1-y_2)\\ & x_1 \ge (1-y_1)\\ & x_2 \ge y_2\\ & x_1 + x_2 \ge 3y_3\\ & y_1 + y_2 + y_3 \ge 1\\ & 0 \le x_1, x_2 \le 4\\ & (y_1, y_2, y_3) = (0,1,0)\end{aligned}$$

➥ Upper Bound: $\mathrm{UBD}^2 = 3.5$, $x_1^2 = 1,\ x_2^2 = 1,$ $y_1^2 = 0,\ y_2^1 = 2,\ y_3^2 = 0$

Methods for MINLP with Convex Functions

Outer-Approximation Example

$\xrightarrow{\text{MILP}}$

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y},\eta}\ & \eta \\
\text{s.t.}\ & 4x_1 + y_1 + 1.5y_2 + 0.5y_3 - 4 \le \eta \\
& 3x_1 + 3x_2 + y_1 + 1.5y_2 + 0.5y_3 - 4.5 \le \eta \\
& 2x_1 + 2x_2 + y_1 + 1.5y_2 + 0.5y_3 - 2 \le \eta \\
& -x_2 \le 0 \\
& -x_1 - x_2 + 1.75 \le 0 \\
& -2x_1 - x_2 + 3 \le 0 \\
& x_1 \ge 2y_1 \\
& x_1 - x_2 \le 4(1 - y_2) \\
& x_1 \ge (1 - y_1) \\
& x_2 \ge y_2 \\
& x_1 + x_2 \ge 3y_3 \\
& y_1 + y_2 + y_3 \ge 1 \\
& 0 \le x_1, x_2 \le 4 \\
& y_1, y_2, y_3 \in \{0,1\}
\end{aligned}
$$

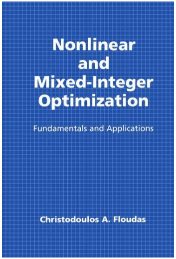
Convergence within 3 iterations

Lower Bound:
$\mathrm{LBD}^3 = 3.5$,
$x_1^3 = 1,\ x_2^3 = 1,\ y_1^3 = 0,$
$y_2^3 = 1,\ y_3^3 = 0$

Contents

Solving MINLPs is challenging in general – We will learn some typical decomposition techniques for MINLPs with either convex or nonconvex participating functions

1. Methods for MINLP with Convex Functions
    - Branch-and-Bound Algorithm
    - Outer-Approximation Algorithm
2. Methods for MINLP with Nonconvex Functions



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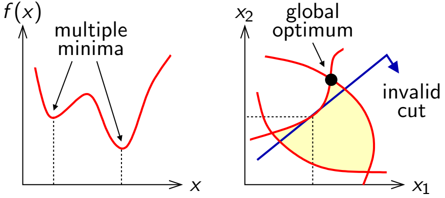
- I.E. Grossmann, Review of nonlinear mixed-integer and disjunctive programming techniques, *Optimization & Engineering* **1**:227-252, 2002

Methods for MINLP with Nonconvex Functions

Main Solution Algorithms

Effects of Nonconvexity:



Heuristic Approaches:

1. Use convex MINLP techniques, assuming valid lower bound
2. Add slacks to the relaxations/ linearizations

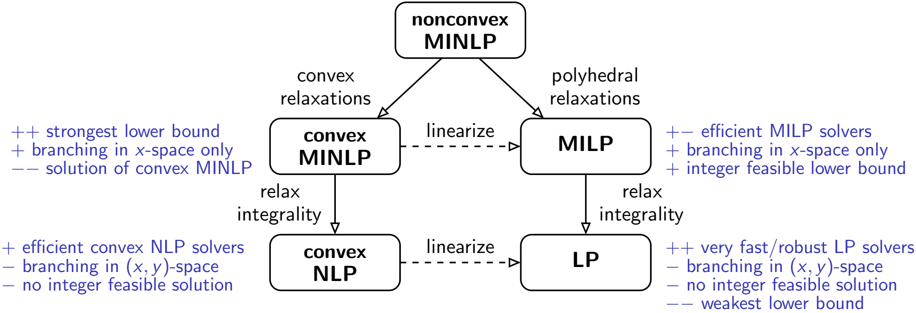
➥ May remain tractable for large-scale nonconvex MINLP!

Rigorous Approaches: Heavily reliant on convex relaxation techniques!

- Gmin-αBB (Adjiman *et al*, 1997, 2000)
- BARON (Ryoo & Sahinidis, 1995; Tawarmalani & Sahinidis, 2002)
- Reformulation/relaxation (Smith & Pantelides, 1999; Zamora & Grossmann, 1999)
- OA for nonconvex MINLP (Kesavan *et al*, 2004)

Methods for MINLP with Nonconvex Functions

Lower-Bounding Techniques



Convex MINLP Relaxation

$$\begin{aligned} \min_{\mathbf{x},\mathbf{y}} \quad & f^{\rm cv}(\mathbf{x}, \mathbf{y}) \\ \text{s.t.} \quad & \mathbf{g}^{\rm cv}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0} \\ & \mathbf{x} \in [\mathbf{x}^{\rm L}, \mathbf{x}^{\rm U}], \ \mathbf{y} \in \{0, 1\} \end{aligned}$$

Convex NLP Relaxation

$$\begin{aligned} \min_{\mathbf{x},\mathbf{y}} \quad & f^{\rm cv}(\mathbf{x}, \mathbf{y}) \\ \text{s.t.} \quad & \mathbf{g}^{\rm cv}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0} \\ & \mathbf{x} \in [\mathbf{x}^{\rm L}, \mathbf{x}^{\rm U}], \ \mathbf{y} \in [0, 1] \end{aligned}$$

Methods for MINLP with Nonconvex Functions

Upper-Bounding Techniques

1. Local Solution of Nonconvex MINLP

   Conceptually straightforward, but:

   - Lacks robustness
   - Comes with high computational burden

2. Local Solution of Nonconvex NLP

   Requires a fixing of binary variables:

   - Solution of convex MINLP/MINLP lower bound
   - Rounding of convex NLP/LP lower bound