# CE4 – 06A
# Advanced Process Optimisation

Lecture 4

## Previous lecture

- Modelling discrete decisions
  - Identify and represent all possible alternatives in superstructures
  - Convert logic relations to algebraic equations
- Mixed Integer Linear Programming (MILP)
- Solution approaches to MILP
  - Brief overview of: (i) Brute Force Approach, (ii) Relaxation and Rounding Approach
  - Description of Branch and Bound (B&B) techniques
    - Basic steps to construct a B&B tree
    - Relaxation properties
    - Branching – node selection strategies
  - Brief mention of cutting planes

# Objectives for today

- Introduction to Mixed Integer Non-Linear Programming (MINLP)
- Understand solution approaches to MINLP
  - Revise basic features of Branch-and-Bound (B&B) techniques
  - Be familiar with Generalized Benders Decomposition (GBD) and Outer-Approximation (OA) algorithms
    - Understand main structure of each algorithm
    - Understand concepts of Primal and Master Problems
  - Be able to apply GBD and OA to an MINLP Process Synthesis example
    - Compare both approaches



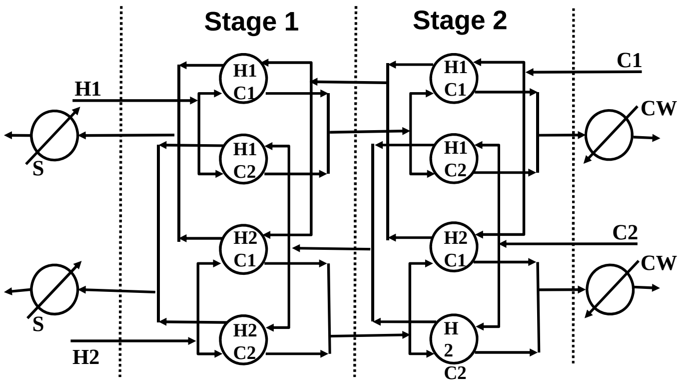
# Mixed Integer Nonlinear Programming (MINLP)

$$\begin{aligned} \min_{\boldsymbol{x},\boldsymbol{y}} \quad & f(\boldsymbol{x},\boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{h}(\boldsymbol{x},\boldsymbol{y}) = 0 \\ & \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) \le 0 \\ & \boldsymbol{x} \in \Re^n \\ & \boldsymbol{y} \in \{0,1\}^q \end{aligned}$$

- $\boldsymbol{x}$: variable vector represents the continuous decisions (flowrates, equipment sizes, pressure, temperature, heat duties)
- $\boldsymbol{y}$: binary variables represent the existence or non-existence of process units
- In an MINLP, at least one function is nonlinear in one variable
- **What solution strategies?**

# Mixed-Integer Non-Linear Programming (MINLP)

<u>Motivating example</u>: Heat Exchanger Network




Assumption: optimal network with minimum utility cost, minimum # of units & minimum area cost for # of units)

<u>But</u> network cost a combination of capital and operating cost → consider both aspect simultaneously in optimal network



# Mixed-Integer Non-Linear Programming (MINLP)

✓ Optimisation problem: find the minimum cost network

✓ Consists of:

- o Binary and continuous variables
- o Linear constraints
- o Nonlinear objective function

⇓

MINLP problem

How do we solve it?

<u>Difficulties</u>

– *combinatorial nature* of the problem (due to *binary variables*)

– presence of *local minima* (due to *nonconvextity* of non-linear functions)

## Nonlinearity in the binary variables

- A nonlinear function of binary variables can always be reformulated so that the binary variables appear linearly

- Examples:
  - o $f = y^2$, with $y \in \{0,1\}$ is equivalent to $f(y) = y$
  - o $f = \exp(y)$, with $y \in \{0,1\}$ is equivalent to $\begin{cases} x = y \\ f = \exp(x) \\ x \in [0,1] \end{cases}$



## "Convex" MINLP

- An oxymoron
- But a useful concept
  - the problem is convex in $x$ for fixed $y$
  - the $y$ variables appear linearly

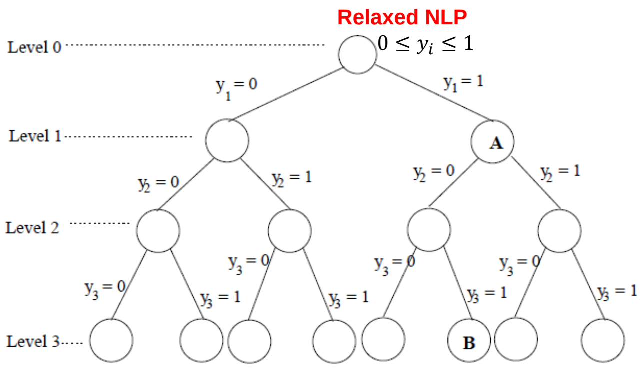
- The algorithms we will see today can solve problems of this type to global optimality

# MINLP: Branch-and-Bound Approaches

- Same principle as in B&B techniques for MILP
- *Main difference* → relaxation at each node is an NLP, not an LP.
- If NLP nonconvex:
  - solution of relaxation can only be a lower bound on MINLP if its global minimum can be identified
  - otherwise, the B&B algorithm may converge to local solution.
- Efficiency:
  - not easy to update the NLPs at each node as in LPs
  - more effort needed at each node
- B&B algorithms can solve problems with integer variables without reformulation.



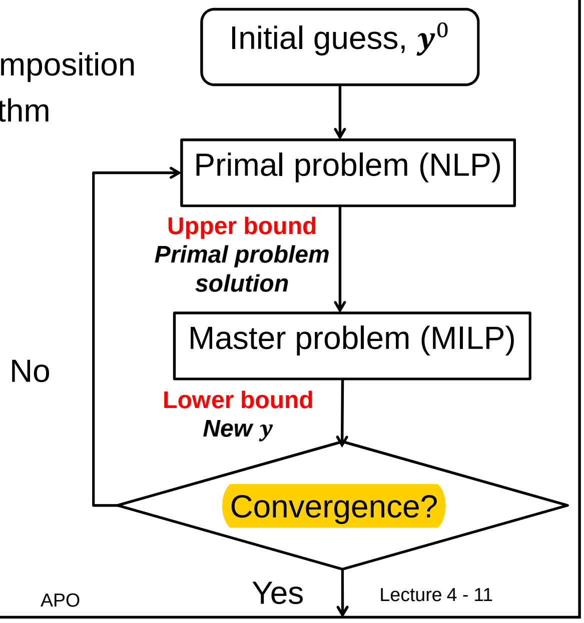
# Branch-and-Bound (B&B) tree



## MINLP: Decomposition Strategies

- Generalized Benders Decomposition
- Outer-Approximation algorithm

- **Basic idea:** Perform separately continuous and discrete optimization






## The Generalized Benders Decomposition (GBD)

- Applied to a class of problems with the following structure (*Geoffrion, 1972*):

$$
\begin{aligned}
\min_{\boldsymbol{x},\boldsymbol{y}} \quad & f^x(\boldsymbol{x}) + \boldsymbol{x}^T A\boldsymbol{y} + c^T\boldsymbol{y} \\
\text{s.t.} \quad & h^x(\boldsymbol{x}) + \boldsymbol{x}^T B\boldsymbol{y} + d^T\boldsymbol{y} = 0 \\
& g^x(\boldsymbol{x}) + \boldsymbol{x}^T C\boldsymbol{y} + e^T\boldsymbol{y} \le 0 \\
& \boldsymbol{x} \in \Re^n \\
& \boldsymbol{y} \in \{0,1\}^q
\end{aligned}
\qquad (GBD)
$$

Notes:

1. Binary variables participate in mixed-bilinear and linear terms.
2. However, any problem of form $(MINLP)$ can be transformed into a $(GBD)$.

GBD algorithm is based on 3 main principles:

1. Partitioning of the variable set
2. Decomposition of the problem
3. Iterative refinement

## GBD – General principles

**Partitioning of the variable set:**

- $\boldsymbol{y}$ variables: complicating variables → handled differently from the $\boldsymbol{x}$ var.
- In original work (*Geoffrion, 1972*), complicating $\boldsymbol{y}$ var not only binary - could also be continuous
- algorithm can also handle bilinear nonconvexities in a rigorous manner.

**Decomposition of the problem:**

- Solve problem considering two types of derived problems:
  - a primal problem → provides an upper bound on the MINLP
  - a master problem → provides a lower bound on the MINLP.

**Iterative refinement:**

- Use information from any given primal and master problems
- Construct new primal and master problems in a way that:
  - obtain tighter bounds
  - achieve convergence within a finite number of iterations



## GBD – The primal problem

**Primal problem**

- $k^{th}$ primal problem $(P^k)$ obtained by fixing the binary variables in $(GBD)$ to some combination $\boldsymbol{y}^k$:

$$\begin{aligned} \min_{\boldsymbol{x},\cancel{\boldsymbol{y}}} \quad & f(\boldsymbol{x},\boldsymbol{y^k}) \\ \text{s.t.} \quad & h(\boldsymbol{x},\boldsymbol{y^k}) = 0 \\ & g(\boldsymbol{x},\boldsymbol{y^k}) \le 0 \\ & \boldsymbol{x} \in \Re^n \end{aligned} \qquad (P^k)$$

where $f(\boldsymbol{x},\boldsymbol{y}) = f^x(\boldsymbol{x}) + \boldsymbol{x^T} A\boldsymbol{y} + c^T\boldsymbol{y}$

$h(\boldsymbol{x},\boldsymbol{y}) = h^x(\boldsymbol{x}) + \boldsymbol{x^T} B\boldsymbol{y} + d^T\boldsymbol{y}$

$g(\boldsymbol{x},\boldsymbol{y}) = g^x(\boldsymbol{x}) + \boldsymbol{x^T} C\boldsymbol{y} + e^T\boldsymbol{y}$

- $(P^k)$: NLP → provides an upper bound on $(GBD)$.
- Solution of $(P^k)$ → NLP feasible or infeasible.

## GBD – Feasible primal problem

- Solution of $(P^k)$ yields an upper bound $\bar{f}^k$ on:
  - the MINLP
  - values of the continuous variables at solution $x^k$
  - values of the optimal Lagrange multipliers at solution $\lambda^k$ and $\mu^k$.

- Based on the optimal solution, the Lagrange function can then be formulated as:

$$\mathcal{L}(x, y; \lambda^k, \mu^k) = f(\boldsymbol{x}, \boldsymbol{y}) + \lambda^{kT} h(\boldsymbol{x}, \boldsymbol{y}) + \mu^{kT} g(\boldsymbol{x}, \boldsymbol{y})$$



## GBD – Infeasible primal problem

**Infeasible Primal problem**

- A feasibility problem is formulated and solved to identify a feasible or nearly feasible point:

$$\begin{aligned} &\min_{\boldsymbol{x},\boldsymbol{\alpha}} \sum_{i=1}^{P} \alpha_i \\ &\text{s.t.}\quad h(\boldsymbol{x}, \boldsymbol{y}^{\boldsymbol{k}}) = 0 \qquad (FP^k) \\ &\qquad g(\boldsymbol{x}, \boldsymbol{y}^{\boldsymbol{k}}) \le 0 \\ &\qquad \boldsymbol{x} \in \Re^n \\ &\qquad \alpha \ge 0 \end{aligned}$$

- Solution of $(FP^k)$ is greater than 0 if no feasible point can be found.
- At solution $x^k$, the Lagrange multipliers $\lambda^{IP,k}$ and $\mu^{IP,k}$ enable the specification of the following Lagrange function:

$$\mathcal{L}(x, y; \lambda^{IP,k}, \mu^{IP,k}) = \lambda^{IP,kT} h(\boldsymbol{x}, \boldsymbol{y}) + \mu^{IP,kT} g(\boldsymbol{x}, \boldsymbol{y})$$

## GBD – The Master problem

- Relaxed master problem at iteration $K$ → constructed from evaluating the Lagrange functions at the solution of primal and infeasible primal for all previous iterations:

$$\begin{aligned} \min_{\boldsymbol{y},\boldsymbol{\eta}^K} \ & \eta^K \\ \text{s.t.} \ & \eta^K \geq \mathcal{L}(\boldsymbol{x^k}, \boldsymbol{y}; \lambda^k, \mu^k), \mathrm{k} = 1, \dots, \mathrm{K} \\ & 0 \geq \mathcal{L}^{IP}(\boldsymbol{x^k}, \boldsymbol{y}; \lambda^{IP,k}, \mu^{IP,k}), \mathrm{k} = 1, \dots, \mathrm{K} \\ & y \in \{0,1\}^q \end{aligned} \qquad (M^k)$$

- $(M^k)$ is an MILP with a single continuous variable
- $\eta^K$ is a lower bound on the solution of $(GBD)$
- new constraint added to $(M^k)$ at each iteration → the sequence of lower bounds is non-decreasing
- $y^K$ can be used to construct the primal problem for iteration $K+1$



## GBD – Integer cuts

### Integer cuts

- Any combination $\boldsymbol{y^k}$ of the binary var should not be generated twice → the following **integer cuts** added to the set of constraints.
  - Let $Z^k = \{i: y_i^k = 0\}$ and $NZ^k = \{i: y_i^k = 1\}$, then:

$$\sum_{i \in NZ^k} y_i - \sum_{i \in Z^k} y_i \leq |NZ^k| - 1$$

  - $|NZ^k|$ cardinality of $NZ^k$
  - $y^k$ becomes an infeasible solution

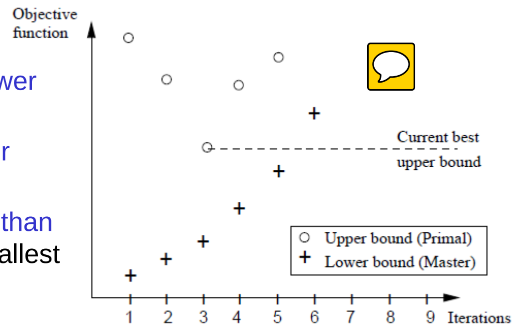
### Example

Build the integer cut for $\boldsymbol{y}^T = (1,0,0,1,1)$

# GBD – Convergence criterion

**Termination criteria**

- Typical progress for the upper and lower bounds during a GBD
- Subsequent solutions → yield a larger objective
- Terminate when lower bound greater than current best upper bound (i.e. the smallest upper bound).




Note:

- When integer cuts added to relaxed master ($M^k$) at each iteration
  - relaxed master may become infeasible before the lower and upper bound converge
    - all feasible integer combinations may have been explored
    - the solution is the best upper bound found so far.



# GBD - Summary

**Standard problem form**

MINLP:
$$z = \min_{x,y} \; f^x(\boldsymbol{x}) + \boldsymbol{x}^T A\boldsymbol{y} + c^T\boldsymbol{y}$$
$$\text{s.t.} \;\; h^x(\boldsymbol{x}) + \boldsymbol{x}^T B\boldsymbol{y} + d^T\boldsymbol{y} = 0$$
$$g^x(\boldsymbol{x}) + \boldsymbol{x}^T C\boldsymbol{y} + e^T\boldsymbol{y} \le 0$$
$$\boldsymbol{x} \in \boldsymbol{X} \subset \Re^n$$
$$\boldsymbol{y} \in \{0,1\}^q$$

Step 1:

a) Set $k = 1$, $z^u = +\infty$,

b) Select $y^1$

Step 2:

a) Solve NLP primal
$$z(y^k) = \min_{x} \; f^x(\boldsymbol{x}) + \boldsymbol{x}^T A y^k + c^T y^k$$
$$\text{s.t.} \;\; h^x(\boldsymbol{x}) + \boldsymbol{x}^T B y^k + d^T y^k = 0$$
$$g^x(\boldsymbol{x}) + \boldsymbol{x}^T C y^k + e^T y^k \le 0$$
$$\boldsymbol{x} \in \boldsymbol{X} \subset \Re^n$$
$$\rightarrow \quad \boldsymbol{x^k}, \boldsymbol{\mu^k}$$

b) If $z(y^k) < z^u$

→ $z^u = z(y^k)$, $x^* = x^k$, $y^* = y^k$

Step 3:

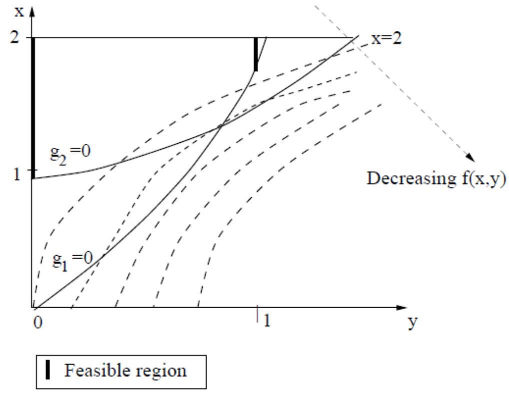
a) Set-up and solve MILP master
$$z^k = \min_{y,\eta} \; \eta^K$$
$$\text{s.t.} \;\; \eta^K \ge \mathcal{L}(\boldsymbol{x^k}, \boldsymbol{y}; \lambda^k, \mu^k), \text{k} = 1, \dots, \text{K}$$
$$0 \ge \mathcal{L}^{IP}(\boldsymbol{x^k}, \boldsymbol{y}; \lambda^{IP,k}, \mu^{IP,k}), \text{k} = 1, \dots, \text{K}$$
$$\sum_{i \in NZ^k} y_i - \sum_{i \in Z^k} y_i \le |NZ^k| - 1$$
$$y \in \{0,1\}^q$$
$$\rightarrow \boldsymbol{y^{k+1}}$$

b) If $z^k \ge z^u$ → stop → Solution $(x^*, y^*, z^u)$

Else, set $k$=$k+1$ → return to step 2 with new $y^{k+1}$

# GBD - Example

$$\begin{aligned} \min_{x,y} \quad & -2.7y + x^2 \\ \text{s.t.} \quad & g_1 = -\ln(1+x) + y \le 0 \\ & g_2 = -\ln(x-0.57) - 1.1 + y \le 0 \\ & 0 \le x \le 2 \\ & y \in \{0,1\} \end{aligned}$$






# Example – Iteration 1

1. Set $y^{(1)} = 1$
2. First primal problem $P^{(1)}$

$$\begin{aligned} \min_{x} \quad & -2.7 + x^2 \\ \text{s.t.} \quad & g_1 = -\ln(1+x) + 1 \le 0 \\ & g_2 = -\ln(x-0.57) - 0.1 \le 0 \\ & 0 \le x \le 2 \end{aligned}$$

Solution: $\left(x^{(1)}, \boldsymbol{\mu}^{(1)}\right) = (1.7183, 9.3417, 0)^T$;   $f = 0.2525$.

Lagrange function:

$$L\left(x^{(1)}, y, \boldsymbol{\mu}^{(1)}\right) = -2.7y + 2.9525 + 9.3417(-1+y)$$

3. Master problem

$$\begin{aligned} \min_{y,\eta^{(1)}} \quad & \eta^{(1)} \\ \text{s.t.} \quad & \eta^{(1)} \ge L(x^{(1)}, y, \mu^{(1)}) \end{aligned}$$

Solution: $\eta^{(1)} = -6.3892$ at $y^{(2)} = 0$

## Example – Iteration 2

1. Second primal problem $P^{(2)}$

$$\begin{aligned} \min_x \quad & x^2 \\ s.t. \quad & g_1 = -\ln(1+x) \le 0 \\ & g_2 = -\ln(x-0.57) - 1.1 \le 0 \\ & 0 \le x \le 2 \end{aligned}$$

Solution: $(x^{(2)}, \boldsymbol{\mu}^{(2)}) = (0.9028, 0, 0.6)^T$; $\quad f = 0.815.$

Higher than best upper bound!

Lagrange function:

$$L(x^{(2)}, y, \boldsymbol{\mu}^{(2)}) = 0.815176 + 0.6y$$

2. Master problem

$$\begin{aligned} \min_{y,\eta^{(2)}} \quad & \eta^{(2)} \\ s.t. \quad & \eta^{(2)} \ge L(x^{(1)}, y, \mu^{(1)}) \\ & \eta^{(2)} \ge L(x^{(2)}, y, \mu^{(2)}) \end{aligned}$$

Solution: $\eta^{(2)} = 0.2525$ at $y^{(3)} = 1$



## The Outer-Approximation (OA)

❖ Applied to a class of problems with the following structure (*Grossmann and coworkers*, 1986 onwards):

$$\begin{aligned} \min_{\boldsymbol{x},\boldsymbol{y}} \quad & f^x(\boldsymbol{x}) + c^T\boldsymbol{y} \\ \text{s.t.} \quad & h^x(\boldsymbol{x}) + d^T\boldsymbol{y} = 0 \\ & g^x(\boldsymbol{x}) + e^T\boldsymbol{y} \le 0 \\ & \boldsymbol{x} \in \Re^n \\ & \boldsymbol{y} \in \{0,1\}^q \end{aligned} \qquad (OA)$$

Professor Ignacio Grossmann will give a seminar at 11am on 24 February in LT3

Notes:

1. Binary variables participate in linear terms only.
2. Any problem of form $(MINLP)$ can be transformed into a $(OA)$.

OA algorithm is based same flowchart as GBD:

- Main difference lies in the formulation of the master problem

## OA – The Master problem

- Relaxed master problem at iteration $K$ → constructed from linearisations at the solution of primal and infeasible primal for all previous iterations:

$$
\begin{aligned}
&\min_{\boldsymbol{x},\boldsymbol{y},\boldsymbol{\eta}^K} \; c^T\boldsymbol{y} + \eta^K \\
&\text{s.t.} \quad \left.\begin{array}{r}
\eta^K \ge f^x(\boldsymbol{x}^k) + \nabla f^x(\boldsymbol{x}^k)^T(\boldsymbol{x}-\boldsymbol{x}^k) \\
T^k\left[\boldsymbol{h}^x(\boldsymbol{x}^k) + \nabla \boldsymbol{h}^x(\boldsymbol{x}^k)^T(\boldsymbol{x}-\boldsymbol{x}^k)\right] + d^T\boldsymbol{y} \le \boldsymbol{0} \\
\boldsymbol{g}^x(\boldsymbol{x}^k) + \nabla - \boldsymbol{g}^x(\boldsymbol{x}^k)^T(\boldsymbol{x}-\boldsymbol{x}^T) + e^T\boldsymbol{y} \le \boldsymbol{0}
\end{array}\right\}, k = 1,\dots,K \qquad (M^k) \\
&\qquad\qquad \boldsymbol{x} \in \mathbb{R}^n \\
&\qquad\qquad \boldsymbol{y} \in \{0,1\}^q
\end{aligned}
$$

- $T^k = (t_{ii}^k)$ is the relaxation matrix

Lagrange multiplier for $h_i^x(\boldsymbol{x}^k)$

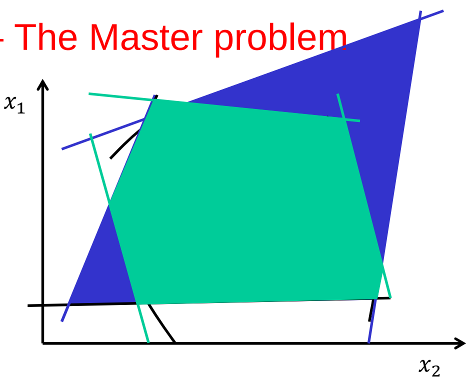
$$
t_{ii}^k = \left\{\begin{pmatrix} -1 \text{ if } \lambda_i^k < 0 \\ +1 \text{ if } \lambda_i^k > 0 \\ 0 \text{ if } \lambda_i^k = 0 \end{pmatrix}\right\}, i = 1, \dots m.
$$

- When the primal problem is infeasible, only the linearisations of the constraints are added to the master



## OA – The Master problem

Graphical interpretation




- As for master problem in GBD, the OA master problem is such that:
  - $\eta^K$ is a lower bound on the solution of $(OA)$
  - new constraint added to $(M^k)$ at each iteration → the sequence of lower bounds is non-decreasing
  - $\boldsymbol{y}^{\boldsymbol{K}}$ can be used to construct the primal problem for iteration $K + 1$

## OA - Summary

MINLP: $z = \min\limits_{x,y} \; f^x(\boldsymbol{x}) + c^T\boldsymbol{y}$

$$\begin{aligned} \text{s.t.}\;\; & h^x(\boldsymbol{x}) + d^T\boldsymbol{y} = 0 \\ & g^x(\boldsymbol{x}) + e^T\boldsymbol{y} \le 0 \\ & \boldsymbol{x} \in \boldsymbol{X} \subset \Re^n \\ & \boldsymbol{y} \in \{0,1\}^q \end{aligned}$$

Step 1:

a) Set $k = 1$, $z^u = +\infty$,

b) Select $y^1$

Step 2:

a) Solve NLP primal

$$z(y^k) = \min_{\boldsymbol{x}} \; f^x(\boldsymbol{x}) + c^T y^k$$

$$\begin{aligned} \text{s.t.}\;\; & h^x(\boldsymbol{x}) + d^T y^k = 0 \\ & g^x(\boldsymbol{x}) + e^T y^k \le 0 \\ & \boldsymbol{x} \in \boldsymbol{X} \subset \Re^n \end{aligned}$$

$\rightarrow \quad \boldsymbol{x^k}, \boldsymbol{\mu^k}$

b) If $z(y^k) < z^u$

$\rightarrow z^u = z(y^k)$, $x^* = x^k$, $y^* = y^k$

Step 3:

a) Set-up and solve MILP master $\rightarrow \boldsymbol{y^{k+1}}$

$$z^k = \min_{y,\eta} \; c^T y + \eta^K$$

$$\text{s.t.} \left.\begin{aligned} & \eta^K \ge f^x(\boldsymbol{x}^k) + \nabla f^x(\boldsymbol{x}^k)^T(\boldsymbol{x} - \boldsymbol{x}^k) \\ & T^k\left[\boldsymbol{h}^x(\boldsymbol{x}^k) + \nabla \boldsymbol{h}^x(\boldsymbol{x}^k)^T(\boldsymbol{x} - \boldsymbol{x}^k)\right] + d^T\boldsymbol{y} \le \boldsymbol{0} \\ & \boldsymbol{g}^x(\boldsymbol{x}^k) + \nabla \boldsymbol{g}^x(\boldsymbol{x}^k)^T(\boldsymbol{x} - \boldsymbol{x}^T) + e^T\boldsymbol{y} \le \boldsymbol{0} \end{aligned}\right\},$$

$$k = 1, \dots, K$$

$$\sum_{i\in NZ^k} y_i - \sum_{i\in Z^k} y_i \le |NZ^k| - 1$$

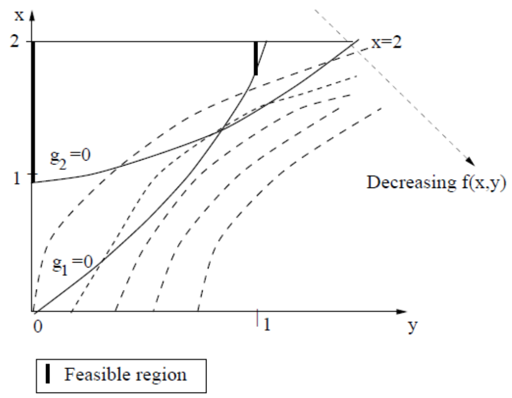
$$y \in \{0,1\}^q$$

b) If $z^k \ge z^u$ → stop → Solution $(x^*, y^*, z^u)$

Else, set $k=k+1$ → return to step 2 with new $y^{k+1}$

## OA – Example revisited

$$\begin{aligned} \min_{x,y} \quad & -2.7y + x^2 \\ s.t. \quad & g_1 = -\ln(1+x) + y \le 0 \\ & g_2 = -\ln(x - 0.57) - 1.1 + y \le 0 \\ & 0 \le x \le 2 \\ & y \in \{0,1\} \end{aligned}$$



## Example – Iteration 1

1. Set $y^{(1)} = 1$
2. First primal problem $P^{(1)}$

$$\begin{aligned} \min_x \quad & -2.7 + x^2 \\ s.t. \quad & g_1 = -\ln(1+x) + 1 \le 0 \\ & g_2 = -\ln(x - 0.57) - 0.1 \le 0 \\ & 0 \le x \le 2 \end{aligned}$$

Solution: $\left(x^{(1)}, \boldsymbol{\mu}^{(1)}\right) = (1.7183, 9.3417, 0)^T$; $\quad f = 0.2525$.

3. Master problem

$$\begin{aligned} \min_{y,\eta^{(1)}} \quad & -2.7y + \eta^{(1)} \\ s.t. \quad & \eta^{(1)} \ge 3.4366x - 2.9526 \\ & -0.3679 - 0.3679x + y \le 0 \\ & 0.2581 - 0.8709x + y \le 0 \\ & 0 \le x \le 2 \\ & y \in \{0,1\} \end{aligned}$$

Solution: $\eta^{(1)} = -1.9339$
at $x = 0.29637$; $y^{(2)} = 0$



## Example – Iteration 2

1. Second primal problem $P^{(2)}$

$$\begin{aligned} \min_x \quad & x^2 \\ s.t. \quad & g_1 = -\ln(1+x) \le 0 \\ & g_2 = -\ln(x - 0.57) - 1.1 \le 0 \\ & 0 \le x \le 2 \end{aligned}$$

Solution: $\left(x^{(2)}, \boldsymbol{\mu}^{(2)}\right) = (0.9028, 0, 0.6)^T$; $\quad f = 0.815$.

Higher than best upper bound!

## Example – Iteration 2

2. Master problem

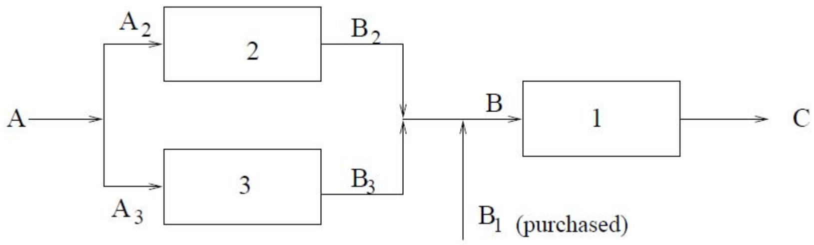
$$
\begin{aligned}
\min_{y,\eta^{(2)}} \quad & -2.7y+\eta^{(2)} \\
s.t. \quad & \eta^{(2)} \geq 3.4366x - 2.9526 \\
& -0.3679-0.3679x+y \leq 0 \\
& 0.2581-0.8709x+y \leq 0 \\
& \eta^{(2)} \geq 1.8056x - 0.8150 \\
& 0.2581-0.8709x+y \leq 0 \\
& 2.7130-2.3256x+y \leq 0 \\
& 0 \leq x \leq 2 \\
& y \in \{0,1\}
\end{aligned}
$$

Solution: $\eta^{(2)} = 0.2525$



## A Process Synthesis Example

- Make chemical C with a process 1 that uses raw material B
- B can be purchased or it can be made with processes 2 or 3, which use A as a raw material
- $F_A$, $F_B$ and $F_C$: flowrates in tons/hr




- What processes and production levels maximise total profit?

# Data

- Conversions:
  - Process 1: $F_C = 0.9F_B$
  - Process 2: $F_B = \ln(1 + F_A)$
  - Process 3: $F_B = 1.2\ln(1 + F_A)$
- Maximum capacity
  - Process 2: 5 tons/hr of B
  - Process 3: 10 tons/hr

Prices:
- A: $1800/ton
- B: $7000/ton
- C: $13000/ton

Maximum demand: 1 ton/hr

**Investment Cost**

| | Fixed cost ($10^3$\$/hr) | Variable cost ($10^3$\$/ton) |
|---|---|---|
| Process 1 | 3.5 | 2.0 |
| Process 2 | 1.0 | 1.0 |
| Process 3 | 1.5 | 1.2 |



# Problem formulation

- What processes and production levels maximise total profit?

- Binary variables:

  $y_1, y_2, y_3$ equal to 1 is corresponding process exists

- Formulation

$$\min_{F,y} -13F_C + 7F_{B1} + 1.8(F_{A2} + F_{A3}) + 3.5(y_1 + 2F_C + y_2 + F_{B2} + 1.5y_3 + 1.2F_{B3})$$

Mass balances

$$F_C = 0.9F_B$$
$$F_{B2} = \ln(1 + F_{A2})$$
$$F_{B3} = 1.2\ln(1 + F_{A3})$$
$$F_B = F_{B1} + F_{B2} + F_{B3}$$

Logical constraints

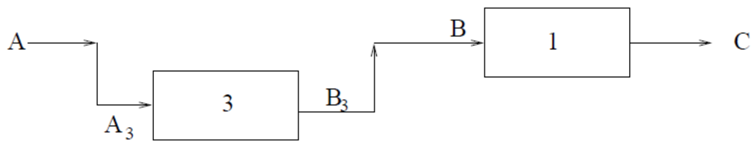
$$F_C \le y_1$$
$$F_{B2} \le 5y_2$$
$$F_{B3} \le 10y_3$$
$$y_2 + y_3 \le 1$$

## Problem solution

- Starting point: $\boldsymbol{y}^T = (1,1,1)$

| Iteration | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| GBD | -27.33 | -23.83 | -11.85 | -2.72 | -1.92 |
| OA/ER | -3.71 | $+\infty$ | — | — | — |

- Solution: $\boldsymbol{y}^T = (1,0,1)$; Profit: $1920 / hr






## GBD vs OA

**GBD**

- Small Master problem, almost purely integer
- Master problem bound not as tight
- More major iterations (NLPs)

**OA**

- Larger Master problem (more constraints and variables, grows rapidly)
- Lower bound at least as tight
- Fewer iterations/NLPs

# Recap

- Three approaches to solve MINLPs
  - Branch-and-Bound
  - Generalized Benders Decomposition
  - Outer-Approximation

- Global optimality guaranteed for “convex” MINLPs
- Comparative analysis of algorithms