

# ECH4905 ChemE Optimization HW 4

Andres Espinosa

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## 1 Problem 1

Consider the following integer programming problem:

$$\begin{aligned} & \text{maximize} && 1.2y_1 + y_2 \\ & \text{subject to} && y_1 + y_2 \leq 1 \\ & && 1.2y_1 + 0.5y_2 \leq 1 \\ & && y_1, y_2 \in \{0, 1\} \end{aligned}$$

### 1.1 Part a

Solve the first relaxed LP subproblem by hand using the simplex method and derive Gomory cuts based on the LP relaxation.

**Solution:** To tackle this problem we first relax the problem and then turn the problem above into the standard form so we can create a simplex tableau from it.

$$\begin{aligned} & \text{maximize} && 1.2y_1 + y_2 \\ & \text{subject to} && y_1 + y_2 + s_1 = 1 \\ & && 1.2y_1 + 0.5y_2 + s_2 = 1 \\ & && y_1 + s_3 = 1 \\ & && y_2 + s_4 = 1 \\ & && y_1, y_2, s_1, s_2, s_3, s_4 \geq 0 \end{aligned}$$

In matrix notation,

$$\begin{aligned} & \text{minimize} && \mathbf{c}^\top \mathbf{x} \\ & \text{subject to} && \mathbf{Ax} = \mathbf{b} \\ & && \mathbf{x} \succeq 0 \end{aligned}$$

where

$$\mathbf{c} = \begin{bmatrix} -1.2 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1.2 & 0.5 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} y_1 \\ y_2 \\ s_1 \\ s_2 \\ s_3 \\ s_4 \end{bmatrix}$$

(with a flipped objective component)

The initial simplex tableau for the problem is as follows:

Basic Var	$y_1$	$y_2$	$s_1$	$s_2$	$s_3$	$s_4$	RHS	$\alpha$
$s_1$	1	1	1	0	0	0	1	
$s_2$	1.2	0.5	0	1	0	0	1	
$s_3$	1	0	0	0	1	0	1	
$s_4$	0	1	0	0	0	1	1	
obj	-1.2	-1	0	0	0	0	-	-

we can define the slack variables equal to the right hand side, and this is in turn a basic feasible solution, so we can jump into phase 2.

We select the  $y_1$  as the entering variable and calculate the alpha value for each basic variable

Basic Var	$y_1$	$y_2$	$s_1$	$s_2$	$s_3$	$s_4$	RHS	$\alpha$
$s_1$	1	1	1	0	0	0	1	$\frac{1}{1}$
$s_2$	1.2	0.5	0	1	0	0	1	$\frac{1}{1.2}$
$s_3$	1	0	0	0	1	0	1	$\frac{1}{1}$
$s_4$	0	1	0	0	0	1	1	$\frac{1}{0}$
obj	-1.2	-1	0	0	0	0	-	-

We pivot this on the 1st column ( $y_1$ ) and the 2nd row ( $s_2$ )

Basic Var	$y_1$	$y_2$	$s_1$	$s_2$	$s_3$	$s_4$	RHS	$\alpha$
$s_1$	0	$\frac{7}{12}$	1	$-\frac{5}{6}$	0	0	$\frac{1}{6}$	
$y_1$	1	$\frac{5}{12}$	0	$\frac{5}{6}$	0	0	$\frac{5}{6}$	
$s_3$	0	$-\frac{5}{12}$	0	$-\frac{5}{6}$	1	0	$\frac{1}{6}$	
$s_4$	0	1	0	0	0	1	1	
obj	0	-0.5	-	-	-	-	-	-

With blands rule, we pick  $y_2$  and calculate the alpha value for each basic variable.

Basic Var	$y_1$	$y_2$	$s_1$	$s_2$	$s_3$	$s_4$	RHS	$\alpha$
$s_1$	0	$\frac{7}{12}$	1	$-\frac{5}{6}$	0	0	$\frac{1}{6}$	$\frac{2}{7}$
$y_1$	1	$\frac{5}{12}$	0	$\frac{5}{6}$	0	0	$\frac{5}{6}$	$\frac{2}{5}$
$s_3$	0	$-\frac{5}{12}$	0	$-\frac{5}{6}$	1	0	$\frac{1}{6}$	$-\frac{1}{5}$
$s_4$	0	1	0	0	0	1	1	$\frac{1}{1}$
obj	0	-0.5	-	-	-	-	-	-

We pivot on the 2nd column ( $y_2$ ) and the 1st row ( $s_1$ ).

Basic Var	$y_1$	$y_2$	$s_1$	$s_2$	$s_3$	$s_4$	RHS	$\alpha$
$y_2$	0	1	$\frac{12}{7}$	$-\frac{10}{7}$	0	0	$\frac{2}{7}$	
$y_1$	1	0	$-\frac{5}{7}$	$\frac{60}{42}$	0	0	$\frac{30}{42}$	
$s_3$	0	0	$\frac{5}{7}$	$-\frac{60}{42}$	1	0	$\frac{12}{42}$	
$s_4$	0	0	$-\frac{12}{7}$	$\frac{60}{42}$	0	1	$\frac{30}{42}$	
obj	0	0	0.857	0.286	0	0	0	-1.143

This is the optimal solution to the LP relaxed problem. Now we will derive Gomory cuts from this LP relaxed problem. Since each constraint has a non-integer solution, we can generate a Gomory cut on each constraint.

$$\begin{aligned}
y_2 + \text{floor}\left(\frac{12}{7}\right)s_1 + \text{floor}\left(\frac{-10}{7}\right)s_2 &\leq \text{floor}\left(\frac{2}{7}\right) \\
y_1 + \text{floor}\left(\frac{-5}{7}\right)s_1 + \text{floor}\left(\frac{10}{7}\right)s_2 &\leq \text{floor}\left(\frac{5}{7}\right) \\
s_3 + \text{floor}\left(\frac{5}{7}\right)s_1 + \text{floor}\left(\frac{-10}{7}\right)s_2 &\leq \text{floor}\left(\frac{2}{7}\right) \\
s_4 + \text{floor}\left(\frac{-12}{7}\right)s_1 + \text{floor}\left(\frac{10}{7}\right)s_2 &\leq \text{floor}\left(\frac{5}{7}\right)
\end{aligned}$$

These turn into the cuts

$$\begin{aligned}
y_2 + s_1 - 2s_2 &\leq 0 \\
y_1 - s_1 + s_2 &\leq 0 \\
s_3 - 2s_2 &\leq 0 \\
s_4 - 2s_1 + s_2 &\leq 0
\end{aligned}$$

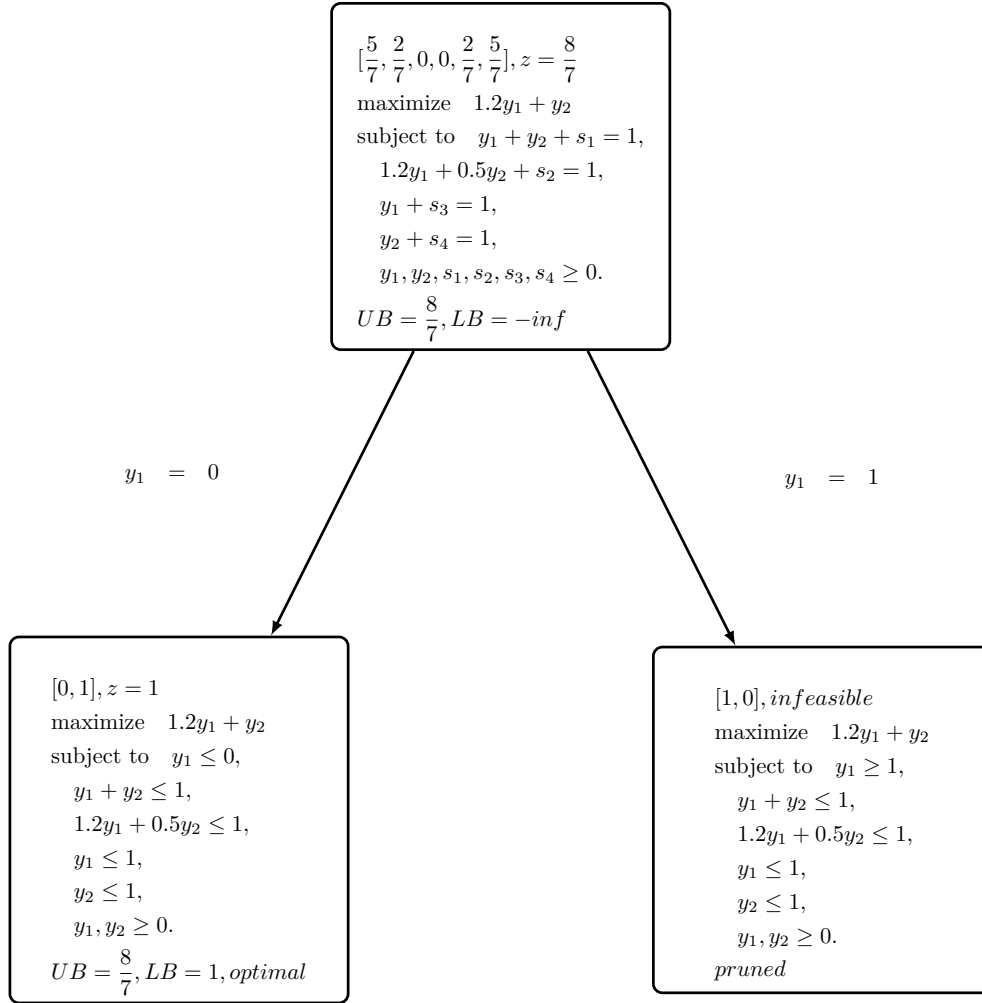
## 1.2 Part b

Solve the above problem with the branch and bound method by enumerating nodes in the tree and solving the LP subproblems using GAMS.

**Solution:** The initial LP relaxed problem is solved in [1.1](#), so we can start with the parent node. An important note for this question, I will be solving the LPs in my custom **gatorpy** LP solver so that I can use them as verification tests. The code used will be available in [section 4.1](#)

$$\begin{aligned}
& \left[\frac{5}{7}, \frac{2}{7}, 0, 0, \frac{2}{7}, \frac{5}{7}\right], z = \frac{8}{7} \\
& \text{maximize} \quad 1.2y_1 + y_2 \\
& \text{subject to} \quad y_1 + y_2 + s_1 = 1, \\
& \quad 1.2y_1 + 0.5y_2 + s_2 = 1, \\
& \quad y_1 + s_3 = 1, \\
& \quad y_2 + s_4 = 1, \\
& \quad y_1, y_2, s_1, s_2, s_3, s_4 \geq 0. \\
& UB = \frac{8}{7}, LB = -inf
\end{aligned}$$

Since all variables are fractional, we can pick the first one  $y_1$  to branch on



Via the branch and bound method, the optimal solution to the problem

$$\begin{aligned} &\text{maximize} && 1.2y_1 + y_2 \\ &\text{subject to} && y_1 + y_2 \leq 1 \\ &&& 1.2y_1 + 0.5y_2 \leq 1 \\ &&& y_1, y_2 \in \{0, 1\} \end{aligned}$$

is  $y_1 = 0, y_2 = 1, z = 1$ .

## 2 Problem 2

Consider the following superstructure for the separation of four chemical components using sharp distillation columns. The total cost of a distillation column is calculated as follows:

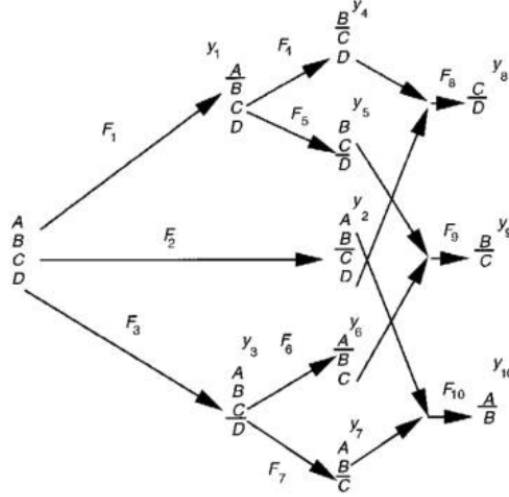


Figure 1: Problem 2 superstructure

$$\text{cost}_k = \alpha_k + \beta_k F_k + \gamma_{\text{Hot}} Q_k^{\text{Hot}} + \gamma_{\text{Cold}} Q_k^{\text{Cold}}$$

where:

- $\alpha_k$  represents a fixed capital cost,
- $\beta_k$  represents the variable investment cost,
- $\gamma_{\text{Hot/Cold}}$  is the cost of hot/cold utilities, and
- $Q_k^{\text{Hot}}/Q_k^{\text{Cold}}$  is the total demand of hot and cold utilities (assumed to be equal).

Given:

- Initial feed: 1000 Kmol/h,
- Feed composition (mole fraction): A = 0.15, B = 0.3, C = 0.35, D = 0.2.

and the following data:

### 2.1 Part A: MILP Formulation

Formulate a Mixed-Integer Linear Programming (MILP) problem to find the optimal sequence of distillation columns. Identify at least 2 logic based equations that can be formulated to tighten the problem formulation.

**Solution:** In order to solve this problem, I will first identify the variables and model the binary flow and decision logic. Then, I will attempt to solve the problem while ignoring the Hot/Cold variables since I am much less confident on implementing that than the other sections. After getting a solution working while ignoring the hot/cold components, I will then implement those  $\gamma, Q$  parameters into the problem.

$k$	Separator	Investment cost		Heat duty coefficients, $K_k$ , ( $10^6$ kJ /kgmol)
		$\alpha_k$ , fixed ( $10^3$ \$/yr)	$\beta_k$ , variable ( $10^3$ \$/hr/kmol yr)	
1	<i>A/BCD</i>	145	0.42	0.028
2	<i>AB/CD</i>	52	0.12	0.042
3	<i>ABC/D</i>	76	0.25	0.054
6	<i>A/BC</i>	125	0.78	0.024
7	<i>AB/C</i>	44	0.11	0.039
4	<i>B/CD</i>	38	0.14	0.040
5	<i>BC/D</i>	66	0.21	0.047
10	<i>A/B</i>	112	0.39	0.022
9	<i>B/C</i>	37	0.08	0.036
8	<i>C/D</i>	58	0.19	0.044

Cost of utilities:

Cooling water	$C_C = 1.3$ ( $10^3$ \$/ $10^6$ kJyr)
Steam	$C_H = 34$ ( $10^3$ \$/ $10^6$ kJyr)

Figure 2: Problem 2 Data

### 2.1.1 Binary logic

To solve this, I will start by creating a series of statements that must be true for this flow to work. I will be using the same  $y$  variables for each distillation column that can be seen in the superstructure diagram 1.

- One of  $y_1, y_2, y_3$  must be chosen.
- If  $y_1$  is chosen, then either  $y_4$  xor  $y_5$  must be chosen.
- If  $y_2$  is chosen, then both  $y_8$  and  $y_{10}$  must be chosen.
- If  $y_3$  is chosen, then either  $y_6$  xor  $y_7$  must be chosen.
- If  $y_4$  is chosen, then  $y_8$  must be chosen.
- If  $y_5$  is chosen, then  $y_9$  must be chosen.
- If  $y_6$  is chosen, then  $y_9$  must be chosen.
- If  $y_7$  is chosen, then  $y_{10}$  must be chosen.

I believe this to be a sufficient set of logic statements to model the problem of choosing a distillation problem. Getting rid of the implications:

- One of  $y_1, y_2, y_3$  must be chosen.
- $y_1 = 0$  or either  $y_4$  xor  $y_5$  must be chosen.
- $y_2 = 0$  or both  $y_8$  and  $y_{10}$  must be chosen.
- $y_3 = 0$  or either  $y_6$  xor  $y_7$  must be chosen.
- $y_4 = 0$  or  $y_8$  must be chosen.

- $y_5 = 0$  or  $y_9$  must be chosen.
- $y_6 = 0$  or  $y_9$  must be chosen.
- $y_7 = 0$  or  $y_{10}$  must be chosen.

We can then translate these second parts into different clauses

One of $y_1, y_2, y_3$ must be chosen.	$\rightarrow$	$y_1 + y_2 + y_3 = 1$
Either $y_4$ xor $y_5$ must be chosen.	$\rightarrow$	$y_4 + y_5 = 1$
both $y_8$ and $y_{10}$ must be chosen.	$\rightarrow$	$y_8 = 1 \cap y_{10} = 1$
Either $y_6$ xor $y_7$ must be chosen.	$\rightarrow$	$y_6 + y_7 = 1$
$y_8$ must be chosen.	$\rightarrow$	$y_8 = 1$
$y_9$ must be chosen.	$\rightarrow$	$y_9 = 1$
$y_9$ must be chosen.	$\rightarrow$	$y_9 = 1$
$y_{10}$ must be chosen.	$\rightarrow$	$y_{10} = 1$

which can in turn be converted to

$$\begin{aligned}
y_1 + y_2 + y_3 &= 1 \\
y_1 &= 0 \cup y_4 + y_5 = 1 \\
y_2 &= 0 \cup (y_8 = 1 \cap y_{10} = 1) \\
y_3 &= 0 \cup y_6 + y_7 = 1 \\
y_4 &= 0 \cup y_8 = 1 \\
y_5 &= 0 \cup y_9 = 1 \\
y_6 &= 0 \cup y_9 = 1 \\
y_7 &= 0 \cup y_{10} = 1
\end{aligned}$$

We can subtract each variable on the left from 1 so we can add them together and distribute the and operation out for the third.

$$\begin{aligned}
y_1 + y_2 + y_3 &= 1 \\
(1 - y_1 = 1) &\cup (((y_4 = 1) \cup (y_5 = 1)) \cap ((1 - y_4 = 1) \cup (1 - y_5 = 1))) \\
((1 - y_2 = 1) \cup (y_8 = 1)) &\cap ((1 - y_2 = 1) \cup (y_{10} = 1)) \\
(1 - y_3 = 1) &\cup (((y_6 = 1) \cup (y_7 = 1)) \cap ((1 - y_6 = 1) \cup (1 - y_7 = 1))) \\
1 - y_3 &= 1 \cup y_6 + y_7 = 1 \\
1 - y_4 &= 1 \cup y_8 = 1 \\
1 - y_5 &= 1 \cup y_9 = 1 \\
1 - y_6 &= 1 \cup y_9 = 1 \\
1 - y_7 &= 1 \cup y_{10} = 1
\end{aligned}$$

We turn this into the equivalent equations

$$\begin{aligned}
y_1 + y_2 + y_3 &= 1 \\
(1 - y_1 = 1) \cup ((y_4 = 1 \cup y_5 = 1)) \\
(1 - y_1 = 1) \cup ((1 - y_4 = 1) \cup (1 - y_5 = 1)) \\
1 - y_2 + y_8 &\geq 1 \\
1 - y_2 + y_{10} &\geq 1 \\
(1 - y_3 = 1) \cup (y_6 = 1 \cup y_7 = 1) \\
(1 - y_3 = 1) \cup ((1 - y_6 = 1) \cup (1 - y_7 = 1)) \\
1 - y_4 + y_8 &\geq 1 \\
1 - y_5 + y_9 &\geq 1 \\
1 - y_6 + y_9 &\geq 1 \\
1 - y_7 + y_{10} &\geq 1
\end{aligned}$$

Finally, we can bring them all into pure math below

$$\begin{aligned}
y_1 + y_2 + y_3 &= 1 \\
1 - y_1 + y_4 + y_5 &\geq 1 \\
1 - y_1 + 1 - y_4 + 1 - y_5 &\geq 1 \\
1 - y_2 + y_8 &\geq 1 \\
1 - y_2 + y_{10} &\geq 1 \\
1 - y_3 + y_6 + y_7 &\geq 1 \\
1 - y_3 + 1 - y_6 + 1 - y_7 &\geq 1 \\
1 - y_4 + y_8 &\geq 1 \\
1 - y_5 + y_9 &\geq 1 \\
1 - y_6 + y_9 &\geq 1 \\
1 - y_7 + y_{10} &\geq 1
\end{aligned}$$

Note: These equations are not completely sufficient on themselves, they require that each distillation column has a positive cost component. Otherwise, it could be possible for  $y_8$  and  $y_7$  to be chosen, but it isn't necessary since the optimization should only yield a solution where distillation columns are used if they are needed to.

## 2.2 Model w/o HotCold

After having solved the binary logic problems above, I will start by denoting the parameters for the model. This model is actually not too bad (unless I am missing the importance of the feed composition asides from flow removal).

*Parameters:* This problem has a feed composition parameter set  $f_A = 0.15, f_B, 0.30, f_C = 0.35, f_D = 0.2$ . (Important note: I am using  $x$  for the flow, so  $f$  is a parameter for feed composition). There is the input supply  $S = 1000$ . Fixed capital cost  $\alpha_k$  for each  $k \in [1, \dots, 10]$  distillation column and variable cost  $\beta_k$ .

*Variables:* I am using the continuous variables  $x_i \in [1, \dots, 13]$  to represent the flow from column to column. Below is a table that maps the variable index to each flow I am also using variables  $y_k, k \in [1, \dots, 10]$  to denote the binary choice of using distillation column  $k$ .



Index	Flow Description
1	Feed to Column 1
2	Feed to Column 2
3	Feed to Column 3
4	Output from Column 1 to Column 4
5	Output from Column 1 to Column 5
6	Output from Column 2 to Column 8
7	Output from Column 2 to Column 10
8	Output from Column 3 to Column 6
9	Output from Column 3 to Column 7
10	Output from Column 4 to Column 8
11	Output from Column 5 to Column 9
12	Output from Column 6 to 9
13	Output from Column 7 to 10

Table 1: Mapping of variable indices to flow descriptions.

*Constraints:* We can model our constraints as follows:

$$\begin{aligned}
& y_k \quad \text{See above for distillation constraints} \\
& x_1, x_4, x_5 \leq Sy_1 \quad \text{BigM Column 1} \\
& x_2, x_6, x_7 \leq Sy_2 \quad \text{BigM Column 2} \\
& x_3, x_8, x_9 \leq Sy_3 \quad \text{BigM Column 3} \\
& x_4, x_{10} \leq Sy_4 \quad \text{BigM Column 4} \\
& x_5, x_{11} \leq Sy_5 \quad \text{BigM Column 5} \\
& x_8, x_{12} \leq Sy_6 \quad \text{BigM Column 6} \\
& x_9, x_{13} \leq Sy_7 \quad \text{BigM Column 7} \\
& x_6, x_{10} \leq Sy_8 \quad \text{BigM Column 8} \\
& x_{11}, x_{12} \leq Sy_9 \quad \text{BigM Column 9} \\
& x_7, x_{13} \leq Sy_{10} \quad \text{BigM Column 10} \\
& x_{13} = \frac{1 - f_c}{1 - f_d} x_9 \text{Column 7 Flow} \\
& x_{12} = \frac{1 - f_a}{1 - f_d} x_8 \text{Column 6 Flow} \\
& x_{11} = \frac{1 - f_d}{1 - f_a} x_5 \text{Column 5 Flow} \\
& x_{10} = \frac{1 - f_b}{1 - f_a} x_4 \text{Column 4 Flow} \\
& x_9 + x_8 = (1 - f_d) x_3 \text{Column 3 Flow} \\
& x_7 = (1 - f_a - f_b) x_2 \text{Column 2 Lower Flow} \\
& x_6 = (1 - f_c - f_d) x_2 \text{Column 2 Upper Flow} \\
& x_5 + x_4 = (1 - f_a) x_1 \text{Column 1 Flow} \\
& x_1 + x_2 + x_3 = S \text{Initial Flow}
\end{aligned}$$

*Objective:* We can model the objective function via components. For brevity, I will just show the component for a general distillation column.

$$z_k = \alpha_k y_k + \beta_k * x_k + heat$$

where  $x_k$  is the entering flow.

### 2.2.1 Tightening constraints

This problem assumes that binary variables will be pushed to zero since they have a positive component in the objective. We can tighten this assumption by introducing constraints that bind parent flows to nested children flows. So, for example,  $x_13$  will not be active if  $x_3$  is not active, however we do not have a constraint that directly models that relationship. We can introduce these two logic-based constraints to tighten the problem:

$$\begin{aligned} 1 - y_3 + y_{10} &\leq 1 \\ 1 - y_2 + y_9 &\geq 1 \end{aligned}$$

## 2.3 Part B: Solve Using GAMS

Solve the problem using GAMS.

**Solution:** A solution was found and summarized in table [2](#). Code is available in section [4.2](#).

## 2.4 Part C: Integer Cut

Once the solution is found:

- Identify the active binary variables in the optimal solution.
- Formulate an integer cut to exclude this solution from the feasible space.
- Solve the problem again to find the next best solution.

I add an integer cut  $y_3 = 0$  and solve to get a worse optimal solution of:

<b>Variable</b>	<b>Value</b>
$z$	581.0000
$x_1$	0
$x_2$	0
$x_3$	1000.0000
$x_4$	0
$x_5$	0
$x_6$	0
$x_7$	0
$x_8$	800.0000
$x_9$	0
$x_{10}$	0
$x_{11}$	0
$x_{12}$	850.0000
$x_{13}$	0
$y_1$	0
$y_2$	0
$y_3$	1
$y_4$	0
$y_5$	0
$y_6$	0
$y_7$	0
$y_8$	1
$y_9$	0
$y_{10}$	0

Table 2: Optimal solution values for the variables.

<b>Variable</b>	<b>Value</b>
$z$	622.0000
$x_1$	0
$x_2$	1000.0000
$x_3$	0
$x_4$	0
$x_5$	0
$x_6$	450.0000
$x_7$	550.0000
$x_8$	0
$x_9$	0
$x_{10}$	0
$x_{11}$	0
$x_{12}$	0
$x_{13}$	0
$y_1$	0
$y_2$	1.0000
$y_3$	0
$y_4$	0
$y_5$	0
$y_6$	0
$y_7$	0
$y_8$	1.0000
$y_9$	0
$y_{10}$	1.0000

Table 3: Summary of problem with integer cut.

### 3 Problem 3

Given are three candidate reactors for the reaction  $A \rightarrow B$ , where we would like to produce 10 kmol/h of  $B$ . Up to 15 kmol/hr of reactant  $A$  are available at a price of \$2/kmol. The data on the three reactors is as follows:

Reactor	Conversion	Cost
1	0.8	$8 + 1.5 \cdot \text{Feed}$
2	0.667	$5.4 + \text{Feed}$
3	0.555	$2.7 + 0.5 \cdot \text{Feed}$

Table 4: Reactor Data

#### 3.1 Part A: Superstructure Design

Design a superstructure to represent this problem.

**Solution:** Not sure if I am oversimplifying this. This superstructure assumes that no  $A$  is recycled

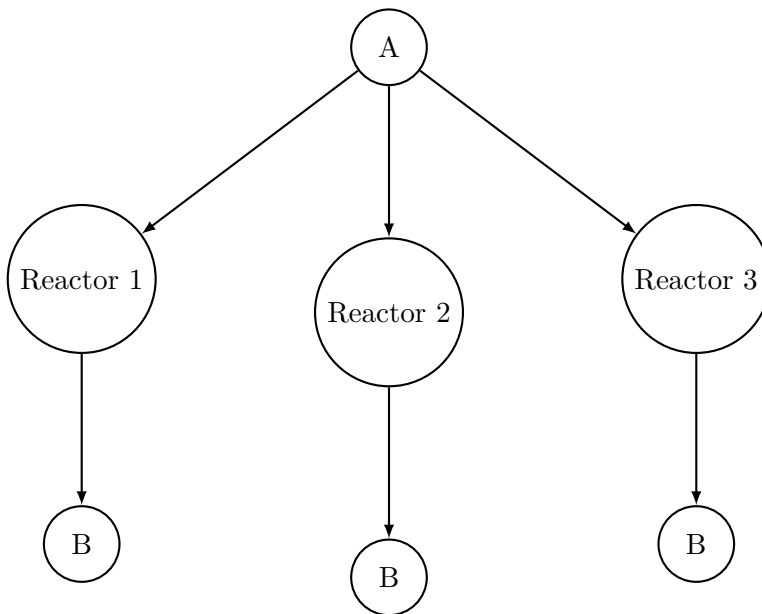


Figure 3: Superstructure for the reaction  $A \rightarrow B$  with three reactors.

back into the reactor, and we only choose one reactor. This is generally a simple problem, we are effectively picking which reactor to use to minimize the cost.

#### 3.2 Part B: MILP Formulation

Determine a MILP formulation.

**Solution:** In order to solve this MILP formulation, I will start thinking about this in a GAMS/modeling language way starting with parameters.

*Parameters:* We have parameters  $k_i$  as the  $A \rightarrow B$  conversion of reactor  $i$ . We also have cost components  $d_i$  as the constant cost of using reactor  $i$  and  $c_i$  as the multiplicative cost of feeding  $A$  through reactor  $i$ . Our demand parameter  $D$  for the amount of  $B$  we would like to produce and

our supply  $S$  that we have available. We can also have the price of using a kmol of  $A$  as  $p$ . Below are the numerical representations of the problem parameters:

$$\begin{aligned} k_1 &= \frac{4}{5}, k_2 = \frac{2}{3}, k_3 = \frac{5}{9} \\ d_1 &= 8, d_2 = 5.4, d_3 = 2.7; c_1 = 1.5, c_2 = 1, c_3 = 0.5 \\ D &= 10, S = 15, p = 2 \end{aligned}$$

*Variables:* Our variables for this problem are as follows: We have  $x_i$  as the amount of  $A$  delivered to the  $i$ -th reactor. In order to model our decision to pick a reactor, we have variables  $y_i$  which are booleans that signify if reactor  $i$  has been chosen.

*Constraints:* We can model our constraints as follows:

$$\begin{aligned} x_i &\leq S, \quad \forall i \in [1, 2, 3] && \text{Supply Constraint} \\ \sum_{i=1}^3 k_i x_i &\geq D && \text{Demand Constraint} \\ \sum_{i=1}^3 y_i &= 1 && \text{One Reactor Constraint} \\ x_i &\leq S y_i, \quad \forall i \in [1, 2, 3] && \text{Big-M One Reactor Flow Constraint} \\ x_i &\geq 0, \quad \forall i \in [1, 2, 3] && \text{Non-negativity} \\ y_i &\in \{0, 1\} \quad \forall i \in [1, 2, 3] && \text{Binaries} \end{aligned}$$

We can also get rid of the supply constraint since the Big-M naturally handles that. The GAMS solution below drops the supply constraint. *Objective:* Our objective in this problem is to minimize the cost while still meeting the demand. We can bunch these costs into different components

$$\begin{aligned} p \sum_{i=1}^3 x_i & \quad \text{Supply component} \\ \sum_{i=1}^3 d_i y_i & \quad \text{Reactor constant component} \\ \sum_{i=1}^3 c_i y_i & \quad \text{Reactor processing component} \end{aligned}$$

### 3.3 Part C: Solve Using GAMS

Solve in GAMS.

**Solution:** The optimal solution was found to be  $x_1 = 12.5, y_1 = 1, z = 34.5$ , and the rest of the variables equal to 0. GAMS code available in section [4.3](#)

## 4 Code

### 4.1 Problem 1 Code

```
# Parameters
A_arr = np.array([[1,1],[1.2,0.5]])
b_arr = np.array([1,1])
c_arr = np.array([1.2,1])
A = Parameter(A_arr)
b = Parameter(b_arr)
c = Parameter(c_arr)
# Variables
y = Variable(2)
# Problem
problem = Problem({
    'maximize': c.T @ y,
    'subject to': [
        A @ y <= b,
        y >= 0,
        y <= 1
    ]
})

# CVX Vars
y_cvx = cp.Variable(2)
# CVX Problem
objective = cp.Maximize(c_arr @ y_cvx)
constraints = [
    A_arr @ y_cvx <= b_arr,
    y_cvx >= 0,
    y_cvx <= 1
]
problem_cvx = cp.Problem(objective, constraints)

get_test_results(problem, problem_cvx, "HW5 Problem 1 initial LP relaxation")
# branch and bound arrays
I_y_1_arr = np.array([[1,0],[0,0]])
I_y_2_arr = np.array([[0,0],[0,1]])
I_y_1 = Parameter(I_y_1_arr)
I_y_2 = Parameter(I_y_2_arr)
# LEFT SPLIT
# Problem
problem = Problem({
    'maximize': c.T @ y,
    'subject to': [
        A @ y <= b,
        y >= 0,
        y <= 1,

```

```

        I_y_1 @ y <= 0,
    ]
})

# CVX Vars
y_cvx = cp.Variable(2)
# CVX Problem
objective = cp.Maximize(c_arr @ y_cvx)
constraints = [
    A_arr @ y_cvx <= b_arr,
    y_cvx >= 0,
    y_cvx <= 1,
    I_y_1_arr @ y_cvx <= 0
]
problem_cvx = cp.Problem(objective, constraints)

get_test_results(problem, problem_cvx, "HW5 Problem 1 Branch and Bound Left Split y_1 <= 0")

# RIGHT SPLIT
# Problem
problem = Problem({
    'maximize': c.T @ y,
    'subject to': [
        A @ y <= b,
        y >= 0,
        y <= 1,
        I_y_1 @ y >= 1,
    ]
})

# CVX Vars
y_cvx = cp.Variable(2)
# CVX Problem
objective = cp.Maximize(c_arr @ y_cvx)
constraints = [
    A_arr @ y_cvx <= b_arr,
    y_cvx >= 0,
    y_cvx <= 1,
    I_y_1_arr @ y_cvx >= 1
]
problem_cvx = cp.Problem(objective, constraints)

get_test_results(problem, problem_cvx, "HW5 Problem 1 Branch and Bound Right Split y_1 >=1")

Test ID: HW5 Problem 1 initial LP relaxation
CVX: (np.float64(1.14), array([[0.71, 0.29]]), True)
GatORPy: (array(1.14285714), array([0.71428571, 0.28571429, 0.
0.71428571]), True)

```



Test passed: False

Test ID: HW5 Problem 1 Branch and Bound Left Split  $y_1 \leq 0$

CVX: (np.float64(1.0), array([[0., 1.]]), True)

GatORPy: (array(1.), array([0., 1., 0., 0.5, 1., 0., 0., 0. ]), True)

Test passed: False

Test ID: HW5 Problem 1 Branch and Bound Right Split  $y_1 \geq 1$

CVX: (None, None, False)

GatORPy: (array(0.8), array([ 1., -0.4, 0.4, 0., 0., 1.4, 0., -1. ]), True)

Test passed: False

## 4.2 Problem 2 Code

GAMS 49.1.0 5c4d4ed6 Feb 15, 2025 DAX-DAC arm 64bit/macOS - 04/14/25 22:09:18 Page  
General Algebraic Modeling System  
Compilation

```
1 * I know this is terribly verbose and I should be using sets
2 * but I haven't been able to get that logic to work
3 Scalars
4 f_a /0.15/
5 f_b /0.30/
6 f_c /0.35/
7 f_d /0.20/
8 S /1000/
9     a_1 / 145 /, b_1 / 0.42 /,
10     a_2 / 52 /, b_2 / 0.12 /,
11     a_3 / 76 /, b_3 / 0.25 /,
12     a_4 / 125 /, b_4 / 0.78 /,
13     a_5 / 44 /, b_5 / 0.11 /,
14     a_6 / 38 /, b_6 / 0.14 /,
15     a_7 / 66 /, b_7 / 0.21 /,
16     a_8 / 112 /, b_8 / 0.39 /,
17     a_9 / 37 /, b_9 / 0.08 /,
18     a_10 / 58 /, b_10 / 0.19 /
19 ;
20 Variables
21 z
22 ;
23 Positive Variables
24 x_1
25 x_2
26 x_3
27 x_4
28 x_5
29 x_6
```

```

30 x_7
31 x_8
32 x_9
33 x_10
34 x_11
35 x_12
36 x_13
37 ;
38 Binary Variables
39 y_1
40 y_2
41 y_3
42 y_4
43 y_5
44 y_6
45 y_7
46 y_8
47 y_9
48 y_10
49 ;
50 Equations
51     bin_constraint_1
52     bin_constraint_2
53     bin_constraint_3
54     bin_constraint_4
55     bin_constraint_5
56     bin_constraint_6
57     bin_constraint_7
58     bin_constraint_8
59     bin_constraint_9
60     bin_constraint_10
61     bin_constraint_11
62     bigm_constraint_1_1
63     bigm_constraint_1_4
64     bigm_constraint_1_5
65     bigm_constraint_2_2
66     bigm_constraint_2_6
67     bigm_constraint_2_7
68     bigm_constraint_3_3
69     bigm_constraint_3_8
70     bigm_constraint_3_9
71     bigm_constraint_4_4
72     bigm_constraint_4_10
73     bigm_constraint_5_5
74     bigm_constraint_5_11
75     bigm_constraint_6_8
76     bigm_constraint_6_12
77     bigm_constraint_7_9

```

```

78     bigm_constraint_7_13
79     bigm_constraint_8_6
80     bigm_constraint_8_10
81     bigm_constraint_9_11
82     bigm_constraint_9_12
83     bigm_constraint_10_7
84     bigm_constraint_10_13
85     flow_constraint_7
86     flow_constraint_6
87     flow_constraint_5
88     flow_constraint_4
89     flow_constraint_3
90     flow_constraint_2_lower
91     flow_constraint_2_upper
92     flow_constraint_1
93     supply_constraint
94     objective_eq
95 ;
96 bin_constraint_1..      y_1 + y_2 + y_3 =e= 1;
97 bin_constraint_2..      1 - y_1 + y_4 + y_5 =g= 1;
98 bin_constraint_3..      1 - y_1 + 1 - y_4 + 1 - y_5 =g= 1;
99 bin_constraint_4..      1 - y_2 + y_8 =g= 1;
100 bin_constraint_5..      1 - y_2 + y_10 =g= 1;
101 bin_constraint_6..      1 - y_3 + y_6 + y_7 =g= 1;
102 bin_constraint_7..      1 - y_3 + 1 - y_6 + 1 - y_7 =g= 1;
103 bin_constraint_8..      1 - y_4 + y_8 =g= 1;
104 bin_constraint_9..      1 - y_5 + y_9 =g= 1;
105 bin_constraint_10..     1 - y_6 + y_9 =g= 1;
106 bin_constraint_11..     1 - y_7 + y_10 =g= 1;
107
108 bigm_constraint_1_1..    x_1  =l= S * y_1;
109 bigm_constraint_1_4..    x_4  =l= S * y_1;
110 bigm_constraint_1_5..    x_5  =l= S * y_1;
111
112 bigm_constraint_2_2..    x_2  =l= S * y_2;
113 bigm_constraint_2_6..    x_6  =l= S * y_2;
114 bigm_constraint_2_7..    x_7  =l= S * y_2;
115
116 bigm_constraint_3_3..    x_3  =l= S * y_3;
117 bigm_constraint_3_8..    x_8  =l= S * y_3;
118 bigm_constraint_3_9..    x_9  =l= S * y_3;
119
120 bigm_constraint_4_4..    x_4  =l= S * y_4;
121 bigm_constraint_4_10..   x_10 =l= S * y_4;
122
123 bigm_constraint_5_5..    x_5  =l= S * y_5;
124 bigm_constraint_5_11..   x_11 =l= S * y_5;
125

```

```

126 bigm_constraint_6_8.. x_8 =l= S * y_6;
127 bigm_constraint_6_12.. x_12 =l= S * y_6;
128
129 bigm_constraint_7_9.. x_9 =l= S * y_7;
130 bigm_constraint_7_13.. x_13 =l= S * y_7;
131
132 bigm_constraint_8_6.. x_6 =l= S * y_8;
133 bigm_constraint_8_10.. x_10 =l= S * y_8;
134
135 bigm_constraint_9_11.. x_11 =l= S * y_9;
136 bigm_constraint_9_12.. x_12 =l= S * y_9;
137
138 bigm_constraint_10_7.. x_7 =l= S * y_10;
139 bigm_constraint_10_13.. x_13 =l= S * y_10;
140
141 flow_constraint_7.. x_13 =e= (1 - f_c) / (1 - f_d) * x_9;
142 flow_constraint_6.. x_12 =e= (1 - f_a) / (1 - f_d) * x_8;
143 flow_constraint_5.. x_11 =e= (1 - f_d) / (1 - f_a) * x_5;
144 flow_constraint_4.. x_10 =e= (1 - f_b) / (1 - f_a) * x_4;
145 flow_constraint_3.. x_9 + x_8 =e= (1 - f_d) * x_3;
146 flow_constraint_2_lower.. x_7 =e= (1 - f_a - f_b) * x_2;
147 flow_constraint_2_upper.. x_6 =e= (1 - f_c - f_d) * x_2;
148 flow_constraint_1.. x_5 + x_4 =e= (1 - f_a) * x_1;
149
150 supply_constraint.. x_1 + x_2 + x_3 =e= S;
151
152 objective_eq..
153 z =e=
154     a_1*y_1 + b_1*x_1 +
155     a_2*y_2 + b_2*x_2 +
156     a_3*y_3 + b_3*x_3 +
157     a_4*y_4 + b_4*x_4 +
158     a_5*y_5 + b_5*x_5 +
159     a_6*y_6 + b_6*x_8 +
160     a_7*y_7 + b_7*x_9 +
161     a_8*y_8 + b_8*(x_6+x_10) +
162     a_9*y_9 + b_9*(x_11+x_12) +
163     a_10*y_10 + b_10*(x_7+x_13);
164
165 Model Superstructure / all /;
166 solve Superstructure using MIP minimizing z;

```

Proven optimal solution

```

MIP Solution:          581.000000      (8 iterations, 0 nodes)
Final Solve:           581.000000      (0 iterations)

```

Best possible: 581.000000  
 Absolute gap: 0.000000  
 Relative gap: 0.000000

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU bin_const~	1.0000	1.0000	1.0000	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bin_const~	-2.0000	.	+INF	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bin_const~	.	-8.88178E-16	+INF	.
---- EQU bin_const~	-2.0000	-2.0000	+INF	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bin_const~	.	1.0000	+INF	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bin_const~	.	.	+INF	.
---- EQU bigm_cons~	-INF	.	.	-0.0100
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	-0.3100
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	-200.0000	.	.
---- EQU bigm_cons~	-INF	-1000.0000	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	-200.0000	.	.
---- EQU bigm_cons~	-INF	-150.0000	.	.
---- EQU bigm_cons~	-INF	.	.	-0.0150
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	-1000.0000	.	.
---- EQU bigm_cons~	-INF	-150.0000	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU bigm_cons~	-INF	.	.	.
---- EQU flow_cons~	.	.	.	.
---- EQU flow_cons~	.	.	.	0.0800
---- EQU flow_cons~	.	.	.	.
---- EQU flow_cons~	.	.	.	.
---- EQU flow_cons~	.	.	.	0.2250
---- EQU flow_cons~	.	.	.	.
---- EQU flow_cons~	.	.	.	.

----	EQU flow_cons~	.	.	.	.
----	EQU supply_co~	1000.0000	1000.0000	1000.0000	0.4300
----	EQU objective~	.	.	.	1.0000
		LOWER	LEVEL	UPPER	MARGINAL
----	VAR z	-INF	581.0000	+INF	.
----	VAR x_1	.	.	+INF	.
----	VAR x_2	.	.	+INF	.
----	VAR x_3	.	1000.0000	+INF	.
----	VAR x_4	.	.	+INF	0.7800
----	VAR x_5	.	.	+INF	0.1100
----	VAR x_6	.	.	+INF	0.3900
----	VAR x_7	.	.	+INF	0.1900
----	VAR x_8	.	800.0000	+INF	.
----	VAR x_9	.	.	+INF	.
----	VAR x_10	.	.	+INF	0.3900
----	VAR x_11	.	.	+INF	0.0800
----	VAR x_12	.	850.0000	+INF	.
----	VAR x_13	.	.	+INF	0.1900
----	VAR y_1	.	.	1.0000	135.0000
----	VAR y_2	.	.	1.0000	-258.0000
----	VAR y_3	.	1.0000	1.0000	76.0000
----	VAR y_4	.	.	1.0000	125.0000
----	VAR y_5	.	.	1.0000	44.0000
----	VAR y_6	.	1.0000	1.0000	38.0000
----	VAR y_7	.	.	1.0000	51.0000
----	VAR y_8	.	.	1.0000	112.0000
----	VAR y_9	.	1.0000	1.0000	37.0000
----	VAR y_10	.	.	1.0000	58.0000

### 4.3 Problem 3 Code

GAMS 49.1.0 5c4d4ed6 Feb 15, 2025 DAX-DAC arm 64bit/macOS - 04/14/25 18:53:07 Page  
 General Algebraic Modeling System  
 Compilation

```

1 SETS
2 i      'set of reactors'      /r1,r2,r3/
3
4 ;
5 Parameters
6 k(i)    'conversion factors'    /r1 0.8, r2 0.666667, r3 0.555555/
7 d(i)    'Reactor constant costs'/r1 8,r2 5.4,r3 2.7/
8 c(i)    'Reactor coeff costs'   /r1 1.5,r2 1,r3 0.5/

```

```

9 ;
10 Scalars
11 De 'Demand' /10/
12 Su 'Supply' /15/
13 pr 'Price' /2/
14 ;
15 Variables
16 z
17 ;
18 Positive Variables
19 x(i)
20 ;
21 Binary Variables
22 y(i)
23 ;
24 Equations
25     demand_constraint
26     one_reactor_constraint
27     flow_constraints(i)
28     objective_eq
29 ;
30 demand_constraint..      sum(i,k(i) * x(i)) =g= De;
31 one_reactor_constraint.. sum(i,y(i)) =e= 1;
32 flow_constraints(i)..    x(i) =l= Su*y(i);
33 objective_eq..          z =e= sum(i,pr*x(i) + d(i) * y(i) + c(i) * y(i));
34
35 Model Superstructure / all /;
36 solve Superstructure using MIP minimizing z;

```

```

COMPILATION TIME      =          0.000 SECONDS          3 MB  49.1.0 5c4d4ed6 DAX-DAC
GAMS 49.1.0 5c4d4ed6 Feb 15, 2025          DAX-DAC arm 64bit/macOS - 04/14/25 18:53:07 Page 2
G e n e r a l   A l g e b r a i c   M o d e l i n g   S y s t e m
Equation Listing      SOLVE Superstructure Using MIP From line 36

```

```

---- demand_constraint  =G=

```

```

demand_constraint..  0.8*x(r1) + 0.666667*x(r2) + 0.555555*x(r3) =G= 10 ; (LHS = 0, INFES = 10)

```

```

---- one_reactor_constraint  =E=

```

```

one_reactor_constraint..  y(r1) + y(r2) + y(r3) =E= 1 ; (LHS = 0, INFES = 1 ****)

```

```

---- flow_constraints  =L=

```

flow\_constraints(r1).. x(r1) - 15\*y(r1) =L= 0 ; (LHS = 0)

flow\_constraints(r2).. x(r2) - 15\*y(r2) =L= 0 ; (LHS = 0)

flow\_constraints(r3).. x(r3) - 15\*y(r3) =L= 0 ; (LHS = 0)

---- objective\_eq =E=

objective\_eq.. z - 2\*x(r1) - 2\*x(r2) - 2\*x(r3) - 9.5\*y(r1) - 6.4\*y(r2) - 3.2\*y(r3) =E= 0 ; (L

GAMS 49.1.0 5c4d4ed6 Feb 15, 2025 DAX-DAC arm 64bit/macOS - 04/14/25 18:53:07 Page 3

General Algebraic Modeling System

Column Listing SOLVE Superstructure Using MIP From line 36

---- z

z

(.L0, .L, .UP, .M = -INF, 0, +INF, 0)  
1 objective\_eq

---- x

x(r1)

(.L0, .L, .UP, .M = 0, 0, +INF, 0)  
0.8 demand\_constraint  
1 flow\_constraints(r1)  
-2 objective\_eq

x(r2)

(.L0, .L, .UP, .M = 0, 0, +INF, 0)  
0.6667 demand\_constraint  
1 flow\_constraints(r2)  
-2 objective\_eq

x(r3)

(.L0, .L, .UP, .M = 0, 0, +INF, 0)  
0.5556 demand\_constraint  
1 flow\_constraints(r3)  
-2 objective\_eq

---- y

y(r1)

(.L0, .L, .UP, .M = 0, 0, 1, 0)



```

      1      one_reactor_constraint
    -15      flow_constraints(r1)
    -9.5      objective_eq

y(r2)
      (.L0, .L, .UP, .M = 0, 0, 1, 0)
      1      one_reactor_constraint
    -15      flow_constraints(r2)
    -6.4      objective_eq

y(r3)
      (.L0, .L, .UP, .M = 0, 0, 1, 0)
      1      one_reactor_constraint
    -15      flow_constraints(r3)
    -3.2      objective_eq

```

Proven optimal solution

```

MIP Solution:      34.500000      (0 iterations, 0 nodes)
Final Solve:      34.500000      (0 iterations)

```

```

Best possible:      34.500000
Absolute gap:      0.000000
Relative gap:      0.000000

```

	LOWER	LEVEL	UPPER	MARGINAL
---- EQU demand_co~	10.0000	10.0000	+INF	2.5000
---- EQU one_react~	1.0000	1.0000	1.0000	.
---- EQU flow_constraints				
	LOWER	LEVEL	UPPER	MARGINAL
r1	-INF	-2.5000	.	.
r2	-INF	.	.	.
r3	-INF	.	.	.
	LOWER	LEVEL	UPPER	MARGINAL
---- EQU objective~	.	.	.	1.0000
	LOWER	LEVEL	UPPER	MARGINAL
---- VAR z	-INF	34.5000	+INF	.
---- VAR x				

	LOWER	LEVEL	UPPER	MARGINAL
r1	.	12.5000	+INF	.
r2	.	.	+INF	0.3333
r3	.	.	+INF	0.6111

---- VAR y

	LOWER	LEVEL	UPPER	MARGINAL
r1	.	1.0000	1.0000	9.5000
r2	.	.	1.0000	6.4000
r3	.	.	1.0000	3.2000

\*\*\*\* REPORT SUMMARY :

0	NONOPT
0	INFEASIBLE
0	UNBOUNDED

EXECUTION TIME = 0.050 SECONDS 4 MB 49.1.0 5c4d4ed6 DAX-DAC

USER: GAMS Demo, for EULA and demo limitations see G250131/0001CB-GEN  
<https://www.gams.com/latest/docs/UG%5FLicense.html> DC0000

\*\*\*\* FILE SUMMARY

Input	/Users/andresespinosa/Documents/GAMS/Studio/workspace/hw5.gms
Output	/Users/andresespinosa/Documents/GAMS/Studio/workspace/hw5.lst