ECH4905 ChemE Optimization HW 4

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1 Problem 1

Consider the following integer programming problem:

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

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.

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

In matrix notation,

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

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	α
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	α
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	α
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	α
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	$\frac{5}{6}$	$\frac{2}{1}$
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	α
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.

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

These turn into the cuts

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

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

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

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

$[\frac{5}{7}, \frac{2}{7}, 0, 0, \frac{2}{7}, \frac{5}{7}], z = \frac{8}{7}$

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

$UB = \frac{8}{7}, LB = -inf$

$y_1 = 0$

$[0, 1], z = 1$

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

$UB = \frac{8}{7}, LB = 1, optimal$

$y_1 = 1$

$[1, 0], infeasible$

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

$pruned$

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

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

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:

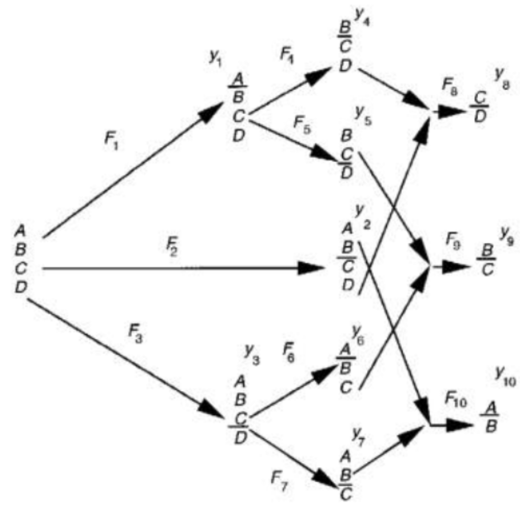

Figure 1: Problem 2 superstructure

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

where:

- α_k represents a fixed capital cost,
- β_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 logicx based equations that can be formulated to tighten the problem formulation.

2.2 Part B: Solve Using GAMS

Solve the problem using GAMS.

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

Cost of utilities:

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

Steam $C_H = 34$ (10^3\$/10^6kJyr)

Figure 2: Problem 2 Data

2.3 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.

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 1: 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

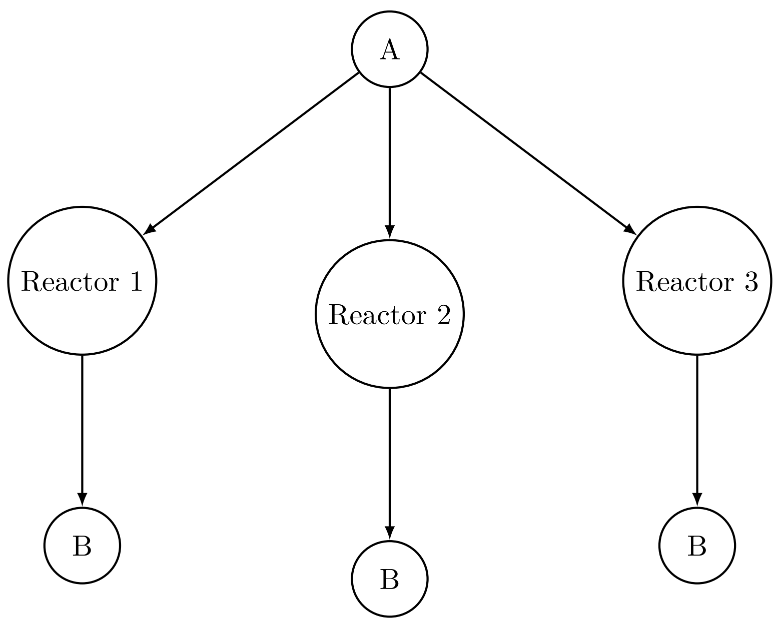

Figure 3: Superstructure for the reaction $A \rightarrow B$ with three reactors.

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:

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

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 4.2

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.        , 0.2857142
       0.71428571]), True)
```

```
Test passed: False

Test ID: HW5 Problem 1 Branch and Bound Left Split y_1 <= 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 >=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 3 Code

```
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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
C o m p i l a t i o n


SETS
i           'set of reactors'       /r1,r2,r3/

;
Parameters
k(i)    'conversion factors'    /r1 0.8, r2 0.666667, r3 0.555555/
d(i)    'Reactor constant costs'/r1 8,r2 5.4,r3 2.7/
c(i)    'Reactor coeff costs'   /r1 1.5,r2 1,r3 0.5/
;
Scalars
De 'Demand' /10/
Su 'Supply' /15/
pr 'Price'  /2/
;
Variables
z
;
Positive Variables
x(i)
;
Binary Variables
y(i)
;
Equations
    demand_constraint
    one_reactor_constraint
    flow_constraints(i)
    objective_eq
;
```

```
  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 ; (LI

GAMS 49.1.0  5c4d4ed6 Feb 15, 2025          DAX-DAC arm 64bit/macOS - 04/14/25 18:53:07 Page 3
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
Column Listing      SOLVE Superstructure Using MIP From line 36


---- z

z
                (.LO, .L, .UP, .M = -INF, 0, +INF, 0)
        1       objective_eq
```

```
---- x

x(r1)
                (.LO, .L, .UP, .M = 0, 0, +INF, 0)
        0.8     demand_constraint
        1       flow_constraints(r1)
       -2       objective_eq

x(r2)
                (.LO, .L, .UP, .M = 0, 0, +INF, 0)
        0.6667  demand_constraint
        1       flow_constraints(r2)
       -2       objective_eq

x(r3)
                (.LO, .L, .UP, .M = 0, 0, +INF, 0)
        0.5556  demand_constraint
        1       flow_constraints(r3)
       -2       objective_eq


---- y

y(r1)
                (.LO, .L, .UP, .M = 0, 0, 1, 0)
        1       one_reactor_constraint
      -15       flow_constraints(r1)
       -9.5     objective_eq

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

y(r3)
                (.LO, .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
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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
```