ECH4905 ChemE Optimization HW 4

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1 Problem 1

Consider the nonlinear program

$$\begin{aligned} \text{minimize} \quad & x_1^2 + 2x_2^2 \\ \text{subject to} \quad & x_1^2 + x_2^2 \le 5 \\ & 2x_1 - 2x_2 = 1 \end{aligned}$$

1.1 Part a

Write the KKT conditions for the problem
Solution: The KKT conditions must satisfy stationarity, complementary slackness, primal feasibility, and dual feasibility. In order to find these conditions, we calculate the following gradients for the stationarity condition

$$\nabla f_0(\mathbf{x}) = \begin{bmatrix} 2x_1 \\ 4x_2 \end{bmatrix}, \quad \nabla f_1(\mathbf{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix}, \quad \nabla g(\mathbf{x}) = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$$

The KKT conditions are then

$$\begin{aligned} \begin{bmatrix} 2x_1 \\ 4x_2 \end{bmatrix} + \lambda \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} + \nu \begin{bmatrix} 2 \\ -2 \end{bmatrix} &= \mathbf{0} \quad \text{Stationarity} \\ \lambda(x_1^2 + x_2^2 - 5) &= 0 \quad \text{Complementary Slackness} \\ x_1^2 + x_2^2 - 5 \le 0, \quad 2x_1 - 2x_2 - 1 &= 0 \quad \text{Primal Feasibility} \\ \lambda &\ge 0 \quad \text{Dual Feasibility} \end{aligned}$$

1.2 Part b

Using 1.1 and other conditions for optimality, what can you conclude about the following solutions to the nonlinear program

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} 1 \\ \frac{1}{2} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} \frac{1}{3} \\ -\frac{1}{6} \end{bmatrix}$$

Solution: For the first point, $\mathbf{x} = [0, 0]$, the primal feasibility is violated because $2(0) - 2(0) - 1 \neq 0$. Therefore, this point is not feasible in the original problem and therefore not optimal.

For the second point, $\mathbf{x} = [1, \frac{1}{2}]$, the following are the KKT conditions

$$\begin{aligned}
\begin{bmatrix}2\\2\end{bmatrix} + \lambda \begin{bmatrix}2\\1\end{bmatrix} + \nu \begin{bmatrix}2\\-2\end{bmatrix} &= \mathbf{0} \quad \text{Stationarity} \\
\lambda(1 + \frac{1}{4} - 5) &= 0 \quad \text{Complementary Slackness} \\
1 + \frac{1}{4} - 5 \leq 0, \quad 2 - 1 - 1 &= 0 \quad \text{Primal Feasibility} \\
\lambda &\geq 0 \quad \text{Dual Feasibility}
\end{aligned}$$

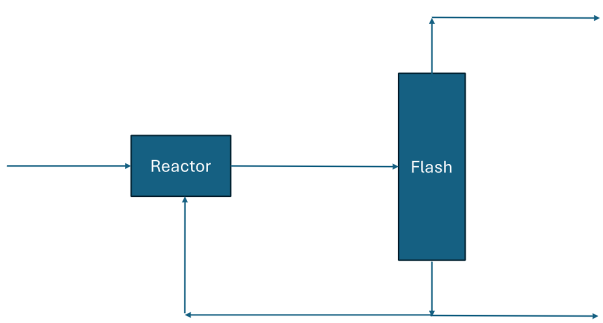
Since $\lambda = 0$ due to the complementary slackness condition, the stationary condition is not satisfied. For the third point, $\mathbf{x} = [\frac{1}{3}, -\frac{1}{6}]$, the following are the KKT conditions

$$\begin{aligned}
\begin{bmatrix}\frac{2}{3}\\-\frac{2}{3}\end{bmatrix} + \lambda \begin{bmatrix}\frac{2}{3}\\-\frac{1}{3}\end{bmatrix} + \nu \begin{bmatrix}2\\-2\end{bmatrix} &= \mathbf{0} \quad \text{Stationarity} \\
\lambda(\frac{1}{9} + \frac{1}{36} - 5) &= 0 \quad \text{Complementary Slackness} \\
\frac{1}{9} + \frac{1}{36} - 5 \leq 0, \quad \frac{2}{3} + \frac{1}{3} - 1 &= 0 \quad \text{Primal Feasibility} \\
\lambda &\geq 0 \quad \text{Dual Feasibility}
\end{aligned}$$

These conditions are satisfied with $\lambda = 0, \nu = -\frac{1}{3}$. Therefore, this point $[\frac{1}{3}, -\frac{1}{6}]$ is an optimal point to the convex optimization problem above.

2 Problem 2

Consider the following flowsheet:



Assume that the following reaction takes place with a 50% conversion. The feed to the reactor consists of pure A.

$$A \rightarrow B$$

The flash separator can be modeled as a perfect separation unit, capable of producing any required purity. We assume that the purge fraction should be between 1% to 99%. The profit is given by the following equation:

$$0.5B_{\text{Top}} - 0.1F_R(500 - T) - 10^{-5}V$$

Where B_{Top} is the molar flow B exiting as top product from the flash separator. And F_R is the recycle molar flow rate.

2.1 Part a

Formulate a model of this process.
Solution: We define the following variables

- F_{A0}: The input flow of A from the left of the reactor.
- F_{AF}: The output flow of A from the bottom of the flash
- F_{AR}: The input flow of A from the recycle stream of the splitter.
- F_{AP}: The output flow of A that is purged to the right of the splitter.
- F_{AI}: The intermediate flow of A from the reactor to the flash.
- F_{BI}: The intermediate flow of B from the reactor to the flash.
- F_{BTop}: The output flow of B from the top of the flash.
- λ: The split fraction of the splitter.
- T: Temperature
- V: Pressure (set to the input flow)

We then have the following optimization problem

$$
\begin{array}{rll}
\text{maximize} & 0.5F_{BTop} - 0.1F_{AR}(500 - T) - 10^{-5}V & \text{Objective} \\
\text{subject to} & F_{A0} + F_{AR} = F_{AI} + F_{BI} & \text{Reactor MB} \\
& F_{AI} + F_{BI} = F_{BTop} + F_{AF} & \text{Flash MB} \\
& F_{AI} = F_{BI} & \text{Reactor Conversion} \\
& F_{BTop} = F_{BI} & \text{Separate flow B} \\
& F_{AI} = F_{AF} & \text{Separate flow A} \\
& F_{AF} = F_{AR} + F_{AP} & \text{Splitter MB} \\
& F_{AR} = \lambda F_{AF} & \text{Recycle Split} \\
& F_{AP} = (1 - \lambda)F_{AF} & \text{Purge Split} \\
& \mathbf{F} \succeq 0 & \text{Non-Negativity} \\
& 0 \leq \lambda \leq 1 & \text{Split Proportion} \\
& 273 \leq T \leq 500 & \text{Temperature Constraints} \\
& V = F_{A0} & \text{Pressure Constraint} \\
& 0.01(F_{AP} + F_{AR}) \leq F_{AP} \leq 0.99(F_{AP} + F_{AR}) & \text{Purge Fraction}
\end{array}
$$

Note that since the split is only two ways, only one variable is used and that avoids an otherwise additional constraint of $\mathbf{1}^\top \lambda = 1$

2.2 Part b

Set up the model in GAMS and try 3 different NLP solvers, compare the results.
Solution: The following code was used to solve the problem. The three solvers used, `baron, gurobi, conopt` resulted in the same answers. Currently, an arbitrary input bound of 1000 is used so that the solver doesnt push the value of the input flow to infinity. I didn't see anything in the problem that naturally constrained the input flow, so I picked a value of 1000.

```
Variables
    profit profit equation;

Positive Variables
    FA0 reactor input of A
    FAF flash output of A
    FAR splitter recycle output of A
    FAP splitter purge output of A
    FAI reactor output of A
    FBI reactor output of B
    FBTop flash output of B
    V pressure
    T temperature
    lambda split fraction;


Equations
    profit_e
    reactor_mb
    flash_mb
    reactor_cons
    sep_B
    sep_A
    split_mb
    recycle_split
    purge_split
    split_prop_l
    temp_l
    temp_g
    pressure
    purge_frac_l
    purge_frac_g
    arbitrary_input_bound;
profit_e.. profit =e= 0.5 * FBTop - 0.1* FAR * (500-T) - 0.00001 * V;

reactor_mb.. FA0 + FAR =e= FAI + FBI;
flash_mb.. FAI + FBI =e= FBTop + FAF;
reactor_cons.. FAI =e= FBI;
sep_B.. FBTop =e= FBI;
sep_A.. FAI =e= FAF;
split_mb.. FAF =e= FAR + FAP;
```

```
recycle_split.. FAR =e= lambda * FAF;
purge_split.. FAP =e= (1-lambda) * FAF;
split_prop_l.. lambda =l= 1;
temp_l.. T =l= 500;
temp_g.. T =g= 273;
pressure.. V =e= FA0;
purge_frac_l.. 0.01* (FAP + FAR) =l= FAP;
purge_frac_g.. FAP =l= 0.99*(FAP + FAR);
arbitrary_input_bound.. FA0 =l= 1000;

Model flowsheet /all/ ;

*option nlp=gurobi;
*option nlp=conopt;
option nlp=baron;

Solve flowsheet using nlp maximizing profit;

Solution      = 495.039504950495  best solution found during preprocessing
Best possible = 495.039504950495
Absolute gap  = 5.6843418860808E-14  optca = 1E-9
Relative gap  = 1.14826025584549E-16  optcr = 0.0001


                           LOWER          LEVEL          UPPER

---- EQU profit_e            .        9.095765E-15         .
---- EQU reactor_mb          .        -2.27374E-13         .
---- EQU flash_mb            .              .              .
---- EQU reactor_c~          .              .              .
---- EQU sep_B               .              .              .
---- EQU sep_A               .              .              .
---- EQU split_mb            .        4.618528E-14         .
---- EQU recycle_s~          .        1.197122E-10         .
---- EQU purge_spl~          .        -1.19703E-10         .
---- EQU split_pro~        -INF            0.9900         1.0000
---- EQU temp_l            -INF          500.0000       500.0000
---- EQU temp_g          273.0000        500.0000         +INF
---- EQU pressure            .              .              .
---- EQU purge_fra~        -INF       -1.23110E-14         .
---- EQU purge_fra~        -INF         -970.2970         .
---- EQU arbitrary~        -INF         1000.0000      1000.0000

                           LOWER          LEVEL          UPPER

---- VAR profit            -INF          495.0395         +INF
---- VAR FA0                 .          1000.0000         +INF
---- VAR FAF                 .           990.0990         +INF
```

```
---- VAR FAR                  .           980.1980         +INF
---- VAR FAP                  .             9.9010         +INF
---- VAR FAI                  .           990.0990         +INF
---- VAR FBI                  .           990.0990         +INF
---- VAR FBTop                .           990.0990         +INF
---- VAR V                    .          1000.0000         +INF
---- VAR T                    .           500.0000         +INF
---- VAR lambda               .             0.9900         +INF
```