ECH4905 ChemE Optimization HW 3

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1 Problem 1

Consider the nonlinear program

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

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

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

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

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

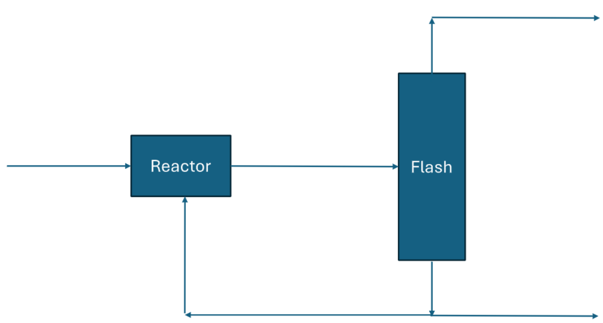
Since $\lambda = 0$ due to the complementary slackness condition, the stationary condition is not satisfied. For the third point, $\mathbf{x} = [\frac{1}{3}, -\frac{1}{6}]$, the following are the KKT conditions

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

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.

$$A \to B$$

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:

2.2 Part b

Set up the model in GAMS and try 3 different NLP solvers, compare the results.
Solution: