# CHBE 552 Problem Set 1

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# 1 Question 1

## 1.1 Part a

$$F(\mathbf{x}) = (x_1 - 2)^4 + (x_1 - 2x_2)^2$$
$$\partial F_{x_1} = 2x_1 - 4x_2 + 4(x_1 - 2)^3$$
$$\partial F_{x_2} = -4x_1 + 8x_2$$

By solving each partial derivative (set equal to zero), the stationaty point is obtained to be

$$\begin{pmatrix} {x_1}^* \\ {x_2}^* \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

The Hessian matrix is determined to be

$$H_a = \begin{bmatrix} 12(x_1 - 2)^2 + 2 & -4 \\ -4 & 8 \end{bmatrix}$$

Then, the Hessian matrix at the stationary point is evaluated to be

$$H_{a,eva.} = \begin{bmatrix} 2 & -4 \\ -4 & 8 \end{bmatrix}$$

The eigen values of the evaluated Hessian matrix are computed to be $0, 10$, thus that stationary point is determined to be a local minimum since the function is Convex at this point.

## 1.2 Part b

$$\begin{aligned} F(\mathbf{x}) &= 2x_1^3 + x_2^2 + x_1^2x_2^2 + 4x_1x_2 + 3 \\ \partial F_{x_1} &= 6x_1^2 + 2x_1x_2^2 + 4x_2 \\ \partial F_{x_2} &= 2x_1^2x_2 + 4x_1 + 2x_2 \end{aligned}$$

By solving each partial derivative (set equal to zero), the stationaty point is obtained to be

$$\begin{pmatrix} {x_1}^* \\ {x_2}^* \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

The Hessian matrix is determined to be

$$H_b = \begin{bmatrix} 12x_1 + 2x_2^2 & 4x_1x_2 + 4 \\ 4x_1x_2 + 4 & 2x_1^2 + 2 \end{bmatrix}$$

Then, the Hessian matrix at the stationary point is evaluated to be

$$H_{b,eva.} = \begin{bmatrix} 0 & 4 \\ 4 & 2 \end{bmatrix}$$

The eigen values of the evaluated Hessian matrix are computed to be $2, -16$, thus that stationary point is determined to be a saddle point.

## 1.3 Part c

$$\begin{aligned} F(x) &= 12x^5 - 45x^4 + 40x^3 + 5 \\ F'(x) &= 60x^4 - 180x^3 + 120x^2 \end{aligned}$$

By solving the first derivative (set equal to zero), the stationaty points are obtained to be

$$x^* = 0, 1, 2$$

The second derivative is determined to be

$$F''(x) = 240x^3 - 540x^2 + 240x$$

Then, the second derivative at the stationary point is evaluated to be

$$F''(x^*) = [0,\ -60,\ 240]$$

By checking the eigen values of the second derivative, those stationary points are determined to be a saddle point ($x = 0$),a local maximun ($x = 1$), and a local minimum ($x = 2$)

# 2 Question 2

## 2.1 Part a

$$\begin{aligned} c = & \frac{58.0555555555556}{T^{0.3017}} + \frac{70.8612328738115T^{0.4925}}{q} \\ & + \frac{2.82512546852169T^{0.7952}}{q} + \frac{19.8593073947553}{q^{0.1899}} \\ & + 8.48356524677597 \cdot 10^{-5} q^{0.671} + 13.9 \\ & + \frac{0.000332994515384452 \cdot (1700.0T + 162.162162162162q)}{q} \end{aligned}$$

The partial derivatives are found to be

$$\begin{aligned} \partial c_q &= -\frac{22.531393600576T^{0.4925}}{q^3} \\ \partial c_T &= -\frac{17.5153611111111}{T^{1.3017}} + \frac{5.54835567414184}{T^{0.5075}q^2} \end{aligned}$$

Since the Hessian matrix of the cost function could be obtained though its complicated and long

So with the implementation of Newton's Method, the optimum tanker size and refinery size are computed to be

$$\begin{aligned} q &= 174833\text{bbl/day} \\ T &= 484726\text{kL} \end{aligned}$$

And the minimun cost of oil is then computed to be

$$c_{\min} = 17.8226$$

Note this result is validated by controlling the initial guess of $q$ and $T$ from a low region $[100, 100]$ and a high region $[1000000, 10000000]$, as well as the region near the given reference $[185000, 485000]$.

By using the reference value of $q$ and $T$, the minimum cost is computed to be

$$c_{\min,ref} = 19.5405$$

## 2.2 Part b

The profit is found to be

$$\begin{aligned} P &= 50 * Yp - \text{cost of additive of A per mol} - \text{cost of steam per mol} \\ &= -2000000S^2 + 0.005Sx_a + 0.047S - 20x_a^2 + 5.0x_a + 1.0 \end{aligned}$$

And the corresponding Hessian matrix are calculated to be

$$H_P = \begin{bmatrix} -40 & 0.005 \\ 0.005 & -4000000 \end{bmatrix}$$

The eigen values are approximated to be $-40$ and $-4000000$, which are both negative. Therefore, the profit function is concave. This conclusion makes sense since it is rational to have a optimum input of material A and steam such that profit is maximized.

## 2.3 Part c

$$\begin{aligned} F = &-14720P + 19.5n(-23PR - 23P + 5000R + 5000)^{0.5} \\ &+ (6560 - 30.2P)(R + 1) \\ &+ 23.2(-23PR - 23P + 5000R + 5000)^{0.62} + 1472000 \end{aligned}$$

$$\nabla F = \begin{bmatrix} -30.2P \\ +\dfrac{19.5n(2500.0 - 11.5P)}{(-23PR - 23P + 5000R + 5000)^{0.5}} \\ +\dfrac{23.2 \cdot (3100.0 - 14.26P)}{(-23PR - 23P + 5000R + 5000)^{0.38}} \\ +6560 \\ 19.5(-23PR - 23P + 5000R + 5000)^{0.5} \\ -30.2R \\ +\dfrac{19.5n(-11.5R - 11.5)}{(-23PR - 23P + 5000R + 5000)^{0.5}} \\ +\dfrac{23.2(-14.26R - 14.26)}{(-23PR - 23P + 5000R + 5000)^{0.38}} \\ -14750.2 \end{bmatrix}$$

Note that the full Hessian matrix is too long to be displayed here, so it is omited. The evaluated form is provided later.

Testpoint is substituted into the gradient of F, and the result is found to be

$$\nabla F_{eva} = \begin{bmatrix} 13739.1885275595 \\ 3052.66879140204 \\ -15764.8373210447 \end{bmatrix}$$

Thus, the optimum do not exist at the reported testpoint.

At that point, the Hessian matrix is evaluated to be

$$H_{F,eva} = \begin{bmatrix} -553.725281183705 & 169.592710633447 & -73.9993400399709 \\ 169.592710633447 & 0 & -12.8922846496965 \\ -73.9993400399709 & -12.8922846496965 & -3.19992471382846 \end{bmatrix}$$

Then the eigenvalues are computed to be $[-609.12, -12.81, 65.02]$.
Therefore, the F function is neither convex nor concave at this test point.

# 3 Question 3

$$W = C_p T_1 \left( \left( \frac{P_2}{P_1} \right)^{\frac{k-1}{k}} + \left( \frac{P_3}{P_2} \right)^{\frac{k-1}{k}} - 2 \right)$$

$$\partial W_{P_2} = C_p T_1 \left( \frac{\left( \frac{P_2}{P_1} \right)^{\frac{k-1}{k}} (k-1)}{P_2 k} - \frac{\left( \frac{P_3}{P_2} \right)^{\frac{k-1}{k}} (k-1)}{P_2 k} \right)$$

By setting the parial derivative of $W$ to zero, the optimal value of $P_2$ is computed to be

$$P_2^* = \left[ -\sqrt{P_1 P_3},\ \sqrt{P_1 P_3} \right]$$

Since pressure can only be a positive value, $P_2$ equals $\sqrt{P_1 P_3}$

Then, the minimum work input is evaluated to be

$$W^* = C_p T_1 \left( \left( \frac{\sqrt{P_1 P_3}}{P_1} \right)^{\frac{k-1}{k}} + \left( \frac{P_3}{\sqrt{P_1 P_3}} \right)^{\frac{k-1}{k}} - 2 \right)$$

# 4 Question 4

$$u = 4\varepsilon \left( -\frac{\sigma^6}{r^6} + \frac{\sigma^{12}}{r^{12}} \right)$$

$$\frac{\partial u}{\partial r} = 4\varepsilon \left( \frac{6\sigma^6}{r^7} - \frac{12\sigma^{12}}{r^{13}} \right)$$

$$\frac{\partial^2 u}{\partial r^2} = 4\varepsilon \left( -\frac{42\sigma^6}{r^8} + \frac{156\sigma^{12}}{r^{14}} \right)$$

Stationary Points are computed to be

$$r^* = \left[ -\sqrt[6]{2}\sigma,\ \sqrt[6]{2}\sigma \right]$$

Note, only real solutions remains to be tested. Substitute those $r^*$ values into the second partial derivative of u to obtain

$$\begin{aligned}\frac{\partial^2 u}{\partial r^2}\Big|_{r_1} &= \frac{36 \cdot 2^{\frac{2}{3}}\varepsilon}{\sigma^2} \\ \frac{\partial^2 u}{\partial r^2}\Big|_{r_2} &= \frac{36 \cdot 2^{\frac{2}{3}}\varepsilon}{\sigma^2}\end{aligned}$$

Since second partial derivative of $u$ are evaluated to be positive at both of the stationary points when $e$ and $\sigma$ are both positive, one can conclude that, both of those stationary points are local minimum.

Thus, at the stationary points, the magintude of potential energy is evaluated to be

$$u^* = -e$$

# 5 Question 5

## 5.1 Part a

$$\begin{aligned}F_a &= x_1^4 - 15x_1^2 + 12x_2^3 - 56x_2 + 60 \\ \partial F_{a,x_1} &= 4x_1^3 - 30x_1 \\ \partial F_{a,x_2} &= 36x_2^2 - 56 \\ H_a &= \begin{bmatrix} 12x_1^2 - 30 & 0 \\ 0 & 72x_2 \end{bmatrix} \\ [x_1^*, x_2^*] &= \Big[ \left(0, -\frac{\sqrt{14}}{3}\right), \left(0, \frac{\sqrt{14}}{3}\right), \left(-\frac{\sqrt{30}}{2}, -\frac{\sqrt{14}}{3}\right), \\ &\quad \left(-\frac{\sqrt{30}}{2}, \frac{\sqrt{14}}{3}\right), \left(\frac{\sqrt{30}}{2}, -\frac{\sqrt{14}}{3}\right), \left(\frac{\sqrt{30}}{2}, \frac{\sqrt{14}}{3}\right)\Big]\end{aligned}$$

After test for eigen values of of Hessian matric evaluated at each stationary point, they are identified as below

$$\begin{aligned}
&[\left(\left(0, -\frac{\sqrt{14}}{3}\right), \text{Negative definite (local maximum)}\right), \\
&\left(\left(0, \frac{\sqrt{14}}{3}\right), \text{Indefinite (saddle point)}\right), \\
&\left(\left(-\frac{\sqrt{30}}{2}, -\frac{\sqrt{14}}{3}\right), \text{Indefinite (saddle point)}\right), \\
&\left(\left(-\frac{\sqrt{30}}{2}, \frac{\sqrt{14}}{3}\right), \text{Positive definite (local minimum)}\right), \\
&\left(\left(\frac{\sqrt{30}}{2}, -\frac{\sqrt{14}}{3}\right), \text{Indefinite (saddle point)}\right), \\
&\left(\left(\frac{\sqrt{30}}{2}, \frac{\sqrt{14}}{3}\right), \text{Positive definite (local minimum)}\right)]
\end{aligned}$$

## 5.2 Part b

$$\begin{aligned}
F_b &= x_1^2 - 4x_1x_2 + x_2^2 + x_3^2 \\
\partial F_{b,x_1} &= 2x_1 - 4x_2 \\
\partial F_{b,x_2} &= -4x_1 + 2x_2 \\
\partial F_{b,x_3} &= 2x_3 \\
H_b &= \begin{bmatrix} 2 & -4 & 0 \\ -4 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \\
[x_1^*, x_2^*, x_3^*] &= \{x_1 : 0,\ x_2 : 0,\ x_3 : 0\}
\end{aligned}$$

After test for eigen values of of Hessian matric evaluated at that stationary point,it is determined to be a saddle point.

# 6 Question 6

$$F = (1 - x_1)^2 + 100\left(-x_1^2 + x_2\right)^2$$
$$\nabla F = \begin{bmatrix} -400x_1\left(-x_1^2 + x_2\right) + 2x_1 - 2 \\ -200x_1^2 + 200x_2 \end{bmatrix}$$
$$H_F = \begin{bmatrix} 1200x_1^2 - 400x_2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

At $[1, 1]$, the gradient of F and Hessian matrix of F are evaluated to be

$$\nabla F \mid_{\mathbf{x}^*} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
$$H_F \mid_{\mathbf{x}^*} = \begin{bmatrix} 802 & -400 \\ -400 & 200 \end{bmatrix}$$

The eigen values of Hessian matrix of F evaluated at this point is computed to be

$$\left\{501 - \sqrt{250601},\ \sqrt{250601} + 501\right\}$$

Both of eigenvalues are positive, thus, $\mathbf{x}^*$ is indeed a strong local minimum.

By setting the gradient of F to zero, the stationary point is solved to be $[1, 1]$, which is the same as indicated in part b.

Since in part b that stationary point is prooved to be a strong local minimum, thus the function F is convex at that point.