CE3-08 – Process Model Solution and Optimization

Problem Sheet for Topic #3

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1. Check whether the following functions are convex or concave over the domains specified using the Hessian test. Try to plot the functions in Matlab to validate your answers.

   (a) $f(x) = x\sin(x)$, for $x \in [0, \pi]$? for $x \in [\frac{\pi}{2}, \pi]$?

   (b) $f(x_1, x_2) = 1000 + 7x_1 - 700x_2 + 23x_1x_2 + 10x_1^2 + 5.6x_2^2$, for $x_1, x_2 \in \mathbb{R}$?

   (c) $f(x_1, x_2) = \dfrac{10}{\sqrt{x_1}} - \log(x_2)$, for $x_1, x_2 > 0$?

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2. For each of the following functions, determine *analytically* whether the specified $\mathbf{x}$ is: (i) definitely a local minimum; (ii) possibility a local minimum; (iii) definitely a local maximum; and/or (iv) possible a local maximum. Try to validate your answers graphically.

   (a) $f(x_1, x_2) = 12x_2 - (x_1)^2 + 3x_1x_2 - 3(x_2)^2$, at $\mathbf{x} = (12, 8)$?

   (b) $f(x_1, x_2) = 4(x_1)^2 + \dfrac{3}{x_2} - 8x_1 + 3x_2$, at $\mathbf{x} = (1, 1)$?

   (c) $f(x_1, x_2) = (x_1)^3(x_2)^2$, at $\mathbf{x} = (0, 0)$?

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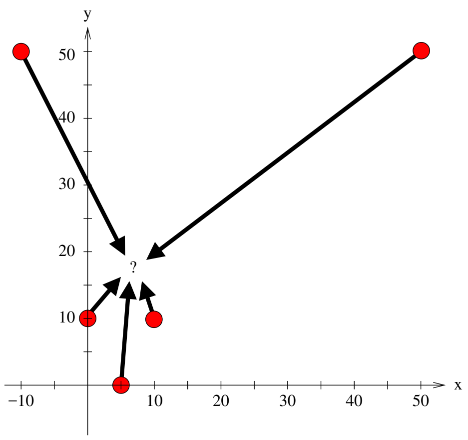
3. It is desired to connect five oil wells to a single collection point using the minimum total length of pipe, as shown in the figure below. Each pipe segment will be placed in straight line from the well to the collection point.



The locations of the oil wells in the (x, y)-plane are the following:

- $(x_1, y_1) = (5, 0)$
- $(x_2, y_2) = (0, 10)$
- $(x_3, y_3) = (10, 10)$
- $(x_4, y_4) = (50, 50)$
- $(x_5, y_5) = (-10, 50)$

   (a) Formulate an (unconstrained) NLP model that can be used to determine where the collection point should be located in the plane.

   (b) Could this problem exhibit multiple local optima? Justify your answer.

   (c) Implement this problem in Matlab and solve it using the fminunc function. In particular:

- ◦ try to provide the gradient of the objective function (see option GradObj)
- ◦ set the termination tolerances on the variables and the objective gradient value to 1e-7 (options TolX and TolFun)
- ◦ select a 'good' initial guess (e.g., the origin $(0, 0)$)

Report the optimal point and solution value found by fminunc, as well as the termination flag, total number of iterations, and measure of first-order optimality. Plot the objective function and compare the actual maximum with the numerical solution.

(d) Repeat Question 3c using GAMS instead of MATLAB.

(e) Check that the first- and second-order necessary conditions for optimality are satisfied at the optimum point found previously.

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4. Consider the following QP problem:

$$
\begin{aligned}
\min_{\mathbf{x}}\ & x_1^2 + x_2^2 - 8x_1 - 16x_2 + 32 \\
\text{s.t. } & x_1 + x_2 \leq 5 \\
& x_1 \geq 0
\end{aligned}
$$

(a) Write down the KKT conditions for this QP. Identify such KKT points, by successively considering *all* possible active sets (4 possibilities).

(b) Check whether the QP is convex. Conclude.

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5. In this question, you are to develop and test an implementation of the active-set method for QP optimization, as described on Slide #63 of Lecture 3. Your function will comply with the following:

qp.m

```
function [xopt, fopt] = qp( c, Q, Ae, be, Ai, bi )

  % <- TO BE COMPLETED

end
```

The input arguments of this function are as follows:

- `c` , the linear part of the objective function
- `Q`, the quadratic part of the objective function
- `Ae`, the coefficient matrix of equality constraints
- `be`, the right-hand-side vector of equality constraints
- `Ai`, the coefficient matrix of inequality constraints
- `bi`, the right-hand-side vector of inequality constraints

On successful completion, `xopt` and `fopt` should contain, respectively, an (approximate) optimum point and the corresponding solution value.

(a) Develop the m-file `qp.m` in order to implement the implementing to active-set method, in the case of a minimization problem. Make sure to test that the QP is convex inside the function.

(b) Debug and test your m-file by considering the same problem as in Question 4 above.

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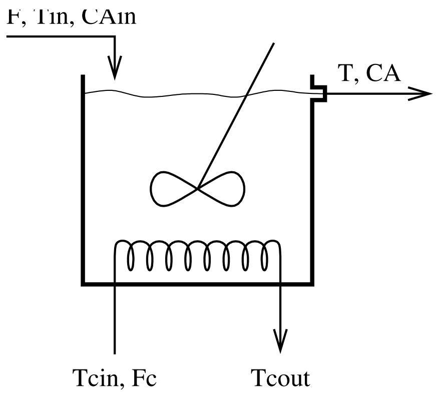
6. Consider the isothermal, constant volume CSTR with series reaction $\mathsf{A} \xrightarrow{k_1} \mathsf{B} \xrightarrow{k_2} \mathsf{C}$ shown in the figure below. Our goal is to maximize the concentration of species B, C_{B}, by adjusting the flow rate F and inlet concentration $C_{\mathsf{A}}^{\text{in}}$ simultaneously, while keeping all other variables and parameters constant (see table below). Both manipulated variables F and $C_{\mathsf{A}}^{\text{in}}$ should be nonnegative and their maximum allowable levels are F_U and $C_{\mathsf{A}}^{\text{in,U}}$, respectively.



Param.	Value	
k_1	5.0	min^{-1}
k_2	2.0	min^{-1}
V	1.0	L
C_{A}^{U}	0.2	mol L^{-1}
$C_{\mathsf{A}}^{\text{in},U}$	1.0	mol L^{-1}
F^{U}	20.0	L min^{-1}

Figure 1: CSTR with series reaction and problem data.

(a) This optimization problem is first modeled as the following constrained NLP:

$$\boxed{\begin{aligned}
\max_{F, C_{\mathsf{A}}^{\text{in}}} \quad & C_{\mathsf{A}}^{\text{in}} \frac{F k_1 V}{(F + k_1 V)(F + k_2 V)} \\
\text{s.t.} \quad & C_{\mathsf{A}}^{\text{in}} \frac{F}{F + k_1 V} \leq C_{\mathsf{A}}^{U} \\
& 0 \leq F \leq F^{U} \\
& 0 \leq C_{\mathsf{A}}^{\text{in}} \leq C_{\mathsf{A}}^{\text{in},U}
\end{aligned}}$$

i. Implement this optimization problem in Matlab, then solve it using the fmincon function, starting from the initial values $F = 10$ L min^{-1}, $C_{\mathsf{A}}^{\text{in}} = 0.5$ mol L^{-1}. Check that the solver terminated successfully. Report the optimal point and solution value found by fmincon, as well as the optimal active set. Comment.

Indications. Use finite difference approximations for the gradients of the objective and constraint functions for simplicity (see options GradObj and GradCon); set the termination tolerances on the variables, constraints and KKT conditions value to 1e-7 (options TolX TolCtr and TolFun).

ii. Repeat Question 6(a)i using GAMS instead of MATLAB. Comapre the results.

Indications. GAMS allows a user to fix the activity levels (values) of variables through the `.l` suffix:

```
VARIABLE x1;
x1.l = 1.0;
```

assigns the value 1 to the variable `x1`. In particular, values assigned to the variables prior to the `SOLVE` statement serve as initial values for the solver – default values of 0 are used otherwise. This is particularly important for NLP problems. For further information, you can always refer to the GAMS users guide: `http://www.gams.com/dd/docs/bigdocs/GAMSUsersGuide.pdf`.

iii. What is the rate of change in optimal concentration C_{B} for a variation in the maximum allowable concentration C_{A}^U? Using this value (and without any additional calculations in GAMS or MATLAB), estimate the change in C_{B} incurred by increasing C_{A}^U to 0.25 mol L^{-1}.

iv. Modify, then resolve, your GAMS or MATLAB model to reflect the previous change in C_{A}^U. Report the optimal solution value, and compare it to the estimate calculated in the previous question. Discuss your results.

(b) You notice that the same optimization problem could be modeled by incorporating the mole-balance equations directly as equality constraints, thereby yielding the *equivalent* NLP:

$$\boxed{\begin{array}{rl} \displaystyle\max_{F, C_{\mathsf{A}}^{\text{in}}, C_{\mathsf{A}}, C_{\mathsf{B}}} & C_{\mathsf{B}} \\ \text{s.t.} & 0 = F\left(C_{\mathsf{A}}^{\text{in}} - C_{\mathsf{A}}\right) - k_1 C_{\mathsf{A}} V \\ & 0 = -F C_{\mathsf{B}} + \left(k_1 C_{\mathsf{A}} - k_2 C_{\mathsf{B}}\right) V \\ & C_{\mathsf{A}} \leq C_{\mathsf{A}}^U \\ & 0 \leq F \leq F^U \\ & 0 \leq C_{\mathsf{A}}^{\text{in}} \leq C_{\mathsf{A}}^{\text{in},U} \end{array}}$$

i. Repeat Question 6(a)ii for this reformulated optimization model.