National Exams December 2014

Chem – B3, Simulation, Modeling & Optimization

NOTES:

- 1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumption made.
- 2. This is a CLOSED BOOK exam, but candidates may use (a) one of two calculators, the CASIO approved models or SHARP approved models, and (b) a scaled (cm or in) ruler.
- 3. Any five of the seven questions provided constitute a complete paper. If more than five questions are answered, the exam grade will be made up of the five highest marks.

December 2014

- Chem - B3: Simulation, Modeling, & Optimization

Page 1/3

- Q1) Evaporation of water from a lean aqueous NaOH solution is to be carried out in an open top rectangular box shaped tank with a fixed volume of 500 m³. Determine the tank dimensions to minimize the cost of material necessary for the construction of the tank. The sides and the bottoms have the same thickness.
- Q2. In an unconstrained optimization problem the function $f(x) = x^3 7xy + 6y^3$ has to be maximized. (a) Determine if there is, indeed, a maximum, and if yes, at what value of x. (b) Are there other critical (also known as singular) points? If yes, where, and what is their nature?
- Q3) The unsteady state fractional concentration distribution of a compound in a narrow and long channel may be expressed as

$$c/c_0 = 1 - erf\{x/[2(Dt)^{1/2}]\}$$

where c_0 is the constant concentration at the channel inlet (x = 0), D is the dispersion coefficient, and t is time. The error function is defined as

$$\operatorname{erf}(\mathbf{u}) \equiv [2/(\pi)^{1/2}] \int_{0}^{u} \exp(-z^{2}) dz$$

Determine the approximate value of c/c_0 at x = 31 m and t = 3 month, if D = 3 m²/month, and if it is known that at x = 30 m and t = 3 month, $c/c_0 = 0.5230$

Q4.)The growth of a biochemical culture is described by the empirical discrete model

$$y_{k+2}y_{k+1}^{-3/2}=y_k^{-1/2}$$

where y_k is the coded concentration at observation instant k. Using the update operator defined as $E(x_k) \equiv x_{k+1}$, $x_k \equiv \log_a(y_k)$ [a: arbitary logarithm base], determine at what (or between what two consecutive) observation instant(s) will the coded concentration reach the numerical value of 85.

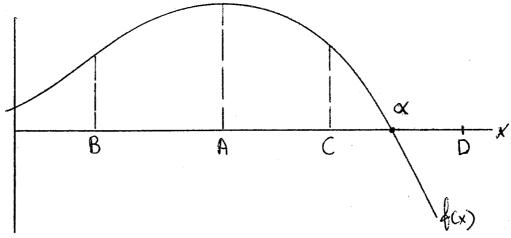
Q5 Ten observation pairs were subjected to linear regression $Y = \beta_0 + \beta_1 x$ and the sample regression parameters $b_0 = -0.8701$; $b_1 = 8.5168$ were obtained by least – squares optimization, along with the following parameters: Total sum of squares = 80.61; Total sum due to regression = 76.87; error variance = 0.468; elements of the $C = (X^T X)^{-1}$ matrix are: $C_{00} = 1.72911$; $C_{01} = C_{10} = -1.28981$; $C_{11} = 0.94354$ [the first column of the X matrix carries ten elements of numerical value 1, the second column carries the ten independent variable values $x_1, x_2, ..., x_{10}$ from top to bottom].(a) Test the hypothesis that Y does not depend on x; (b) Test the hypothesis that regression $Y = \beta_1 x$ can replace the original regression; (c) determine the correlation coefficient (continues on page 2/3).

Page 2/3

Critical T – distribution variates pertinent to this problem, at selected degrees of significance, are below.

α	0.50	0.40	0.30	0.20	0.10
t(α/2)	0.706	0.889	1.108	1.397	1.860

Q6. Given the function f(x) with a single root α [i.e. $f(\alpha) = 0$] shown in the sketch, determine if the root is reached by (a) Newton's method with starting point x = A; (b) Newton's method with starting point x = B; (c) The bisection (also known as interval halving) method with starting interval \overline{AD} ; (d) The bisection method with starting interval \overline{BD} .



Sketch for Q6.

Q7) A small chemical plant is designed to produce x_1 tonne of product A per year, and x_2 tonne of product B per year. The following parameters have been identified by the designers.

Requirement per year	Product A	Product B	
Chemical 1; 180 units available per year	18 units per tonne	3 units per tonne	
Chemical 2; 160 units available per year	40 units per tonne	2 units per tonne	
Labour time*	24 units per tonne	4 units per tonne	

*Agreement with labour unions stipulates that at least 120 labour time units per year be consumed (continues on Page 3/3)

December 2014

- Chem – B3: Simulation, Modeling & Optimization

Page 3/3

- (i) Determine the optimal amounts (tonne per year) of products A and B to be made in the plant to maximize its profit, given that product A sells at 7 MU (monetary unit) per tonne, and product B sells at 4 MU per tonne.
- (ii) Sketch in your answer book [no need to plot!] the feasibility region in the $(x_1;x_2)$ plane, and indicate the position of the optimal operating point.

- END OF EXAM -