Challenge Set 4

Deadline: 2017 at 5pm

Challenge problems are ***optional*** problems for those interested in testing their abilities. For each correct answer to a challenge question, bonus points of 0.1 are given towards the *final overall grade,* i.e., you can potentially earn up to 1.5 points towards the final grade if you get all questions correct. Proper workings must be shown to get any points, and there is no partial credit. Also, because these are bonus questions, instructors will not provide any help or hints (unlike typical problem or practice set questions where generous assistance will be provided) to be fair to all students. Please submit your solutions via the Turnitin assignment "Challenge Set 3" on TED@UCSD (you can simply take a good resolution photo/scan of your solutions with your student ID number and name clearly labelled and convert it to a PDF for upload) by the deadline.

Q1: A catalytic reactor has the following proposed rate equations, where r_A is the rate of the reaction in $\frac{mol}{s}$, C_A is the concentration of reactant A in $\frac{mol}{m^3}$, and k_1, k_2, k_3, and k_4 are rate constants with proper units to make the equations valid.

i. $r_A = \ln\left(k_1 + k_2 {C_A}^2\right)$

ii. $r_A = \frac{k_3 C_A}{k_4 + C_A}$

In lab, the concentration of the reactant and the corresponding rate equation was found at different times. Below is a table showing the collected data.

$r_A\left(\frac{mol}{s}\right)$	2.97	2.88	2.71	2.53	2.16	1.85	1.53	1.21
$C_A\left(\frac{mol}{m^3}\right)$	1.02	0.93	0.78	0.63	0.56	0.41	0.25	0.14

Estimate all four rate constants. Which model better represents the data?

Note: you may check you results using regression calculators, but for full points your solutions should include full work by hand (it may be in a table as done in class).

Solution:

i. $r_A = \ln\left(k_1 + k_2 {C_A}^2\right)$

$e^{r_A} = k_1 + k_2 {C_A}^2$

$y = a + bx$

	X	X^2	Y	Y^2	XY
	1.0404	1.0824	19.49192	379.935	20.27939

	0.8649	0.74805	17.81427	317.348	15.40756
	0.6084	0.37015	15.02928	225.879	9.14381
	0.3969	0.15753	12.55351	157.591	4.98249
	0.3136	0.098345	8.671138	75.18863	2.71927
	0.1681	0.028258	6.359820	40.44730	1.06909
	0.0625	0.003906	4.618177	21.32756	0.28864
	0.0196	0.0003842	3.353485	11.24586	0.06573
Sum	3.4744	2.48902	87.89160	1228.962	53.95598

$$SS_X = \sum X^2 - \frac{(\sum X)^2}{N} = 2.48902 - \frac{12.0715}{8} = 0.98009$$

$$SS_Y = \sum Y^2 - \frac{(\sum Y)^2}{N} = 1228.962 - \frac{7724.9334}{8} = 263.345$$

$$SP = \sum XY - \frac{\sum X \sum Y}{N} = 53.95598 - \frac{305.3706}{8} = 15.7847$$

$$b = \frac{SP}{SS_X} = \frac{15.7847}{0.98009} = 16.10536$$

$$b = k_2 = 16.10536$$

$$a = \bar{Y} - b\bar{X} = 10.98645 - 16.10536 * 0.4343 = 3.99189 = k_1$$

$$r = \frac{SP}{\sqrt{SS_X SS_Y}} = \frac{15.7847}{\sqrt{0.98009 * 263.345}} = 0.98252$$

ii. $r_A = \frac{k_3 C_A}{k_4 + C_A}$

$\frac{1}{r_A} = \frac{k_4 + C_A}{k_3 C_A}$

$\frac{1}{r_A} = \frac{k_4}{k_3}\frac{1}{C_A} + \frac{1}{k_3}$

$y = bx + a$

	X	X^2	Y	Y^2	XY
	0.98039	0.96117	0.33670	0.11337	0.33010
	1.07527	1.15620	0.34722	0.12056	0.37336

	1.28205	1.64366	0.36900	0.13616	0.47308
	1.58730	2.51953	0.39526	0.15623	0.62740
	1.78571	3.18878	0.46296	0.21433	0.82671
	2.43902	5.94884	0.54054	0.29218	1.31839
	4	16	0.65359	0.42719	2.61436
	7.14286	51.02041	0.82645	0.68301	5.90322
Sum	20.29260	82.43859	3.93172	2.14303	12.46662

$$SS_X = \sum X^2 - \frac{(\sum X)^2}{N} = 82.43859 - \frac{411.7896}{8} = 30.96489$$

$$SS_X = \sum Y^2 - \frac{(\sum Y)^2}{N} = 2.14303 - \frac{15.458422}{8} = 0.21073$$

$$SP = \sum XY - \frac{\sum X \sum Y}{N} = 12.46662 - \frac{79.78482}{8} = 2.49352$$

$$b = \frac{SP}{SS_X} = \frac{2.49352}{30.96489} = 0.08053 = \frac{k_4}{k_3}$$

$$a = \bar{Y} - b\bar{X} = 0.491465 - 0.08053 * 2.536575 = 0.28719 = \frac{1}{k_3}$$

$$r = \frac{SP}{\sqrt{SS_X SS_Y}} = \frac{2.49352}{\sqrt{30.96489 * 0.21073}} = 0.97615$$

$$k_3 = 3.48202$$

$$k_4 = k_3 * b = 0.28041$$

Both models have very high correlation coefficients! However, model 1 has a slightly higher correlation coefficient so it better represents the data.

Q2: John is a chemical engineer and has performed an experiment fifty times under different external conditions and formulated the results of the experiment in the table given below. Estimate the mean, median, interquartile range and mode of the following grouped data.

Time taken for completion of the experiment in minutes	Frequency
1-10	8
11-20	14
21-30	12
31-40	9
41-50	7

Solution:

Calculation of mean of the grouped data

Midpoint(**x**)	Frequency **(f)**	**x*f**
5.5	8	44
15.5	14	217
25.5	12	306
35.5	9	319.5
45.5	7	318.5
	Sum=50	1205

Mean =$\frac{1205}{50}$=24.1

Calculation of the median of the grouped data

Frequency is 50 so for median we need to see where 25 lies

Ranges	Frequency	Cumulative Frequency
1-10	8	8
11-20	14	22
21-30	**12**	**34**
31-40	9	43
41-50	7	50

From the cumulative frequency we see that it lies in 21-30 now we need to know where exactly our median is. So we use linear interpolation.

Since intervals are non-overlapping our lower boundary for the class will be average of the upper boundary of previous class and lower boundary of the current class. So Lm= (20+21)/2 =20.5

Median= $\mathbf{20.5 + \frac{(25-22)}{(12)} * 10}$ **= 23.**

Calculation of Q1 and Q3

Q1= $\frac{50}{4} = 12.5$ and Q3= $\frac{3*50}{4}$ = 37.5

Now again we see the CF and find out where these both lie Q1 lies in **2nd** class and Q3 lies in **4th** class.

So we find lower boundary of the class in both classes by averaging upper boundary of the previous class and lower boundary of the current class.

So Lm1=10.5 and Lm3= 30.5

Q1=$10.5 + \frac{12.5-8}{14} * 10$ =13.71

Q3=$30.5 + \frac{37.5-34}{9} * 10$ =34.38

IQR=Q3-Q1=34.38-13.71=**20.67**

Calculation of mode of grouped data

First task is to find out class with highest frequency which is second class here and lower bound is 10.5.

Length of the modal class is 10

We now calculate delta1 and delta2 where delta1 and delta2 are defined as follows

$\text{delta1} = \text{frequency of modal class} - \text{frequnecy of previous class}$

$\text{delta2} = \text{frequency of modal class} - \text{frequnecy of next class}$

Which gives

delta1=14-8=6

delta2=14-12=2

Mode= 10.5+$\frac{6}{6+2} * 10$ =**17.5**

Q3: An article in IEEE Transactions on Instrumentation and Measurement (2001, Vol. 50, pp. 2033–2040) reported on a study that had analyzed powdered mixtures of coal and lime- stone for permittivity. The errors in the density measurement was the response. The data is in the Table below.

i. Fit a multiple linear regression model to these data with the density as the response.
ii. Use the model to predict the density when the dielectric constant is 2.5 and the loss factor is 0.03.

For this analysis, you may choose to use any statistical software of your choice (Excel, Matlab, Python + numpy + scipy + pandas) if you wish, as long as you outline the basic approach in your answer.

Density	*Dielectric Constant*	*Loss factor*
0.749	2.05	0.016
0.798	2.15	0.02
0.849	2.25	0.022
0.877	2.3	0.023
0.929	2.4	0.026
0.963	2.47	0.028
0.997	2.54	0.031
1.046	2.64	0.034
1.133	2.85	0.039
1.17	2.94	0.042
1.215	3.05	0.045