MA4605 Chemometrics Lab C

Part I - Testing for linear dependence. In a laboratory containing polarographic equipment six samples of dust were taken at various distances from the polarograph and the mercury content of each sample was determined. The following results were obtained:

Distance from polarograph,m	1.4,3.8,7.5,10.2,11.7,15.0
Mercury concentration, ng/g	2.4,2.5,1.3,1.3,0.7,1.2

The goal is to examine the possibility that the mercury contamination arose from the polarograph.

Task 1 *Produce a graph of the data representing the dependence of mercury concentration on distance from polarograph. Comment the choice of coordinates.*

Task 2 *Carry out the test if there is any indication of linear dependence between the variables. Comment on the strength of such dependence.* **Task 3** *Add the straight line that best fits the dependence.*

```
Dist = c(1.4,3.8,7.5,10.2,11.7,15.0)
Merc = c(2.4,2.5,1.3,1.3,0.7,1.2)

# compute the correlation coefficient
cor(Dist, Merc)
cor.test(Dist,Merc)

# create a scatterplot
plot(Dist, Merc)

# create a linear model
myModel = lm(Merc~Dist)

summary(myModel)
coef(myModel)

# enhanced scatterplot
plot(Dist, Merc, pch=16, col="red", cex=1.5)
title("Scatterplot")
abline(coef(myModel))

#This adds a line to the scatterplot
```

Part II – Correlation coefficient. The response of a colorimetric test for glucose was checked with the aid of standard glucose solutions. Determine the correlation coefficient from the following data and comment on the result.

Glucose concentration, mM	Absorbance
0	0.002
2	0.150
4	0.294
6	0.434
8	0.570
10	0.704

(Additional for 2012: What is the 95% confidence interval for the correlation coefficient)

```
# Little Trick
# What does this line of code do?

1:5
#and this one?
(1:5)*2


Gluc = c(0,2,4,5,8,10)
Abs1 = c(0.002,0.150,0.294,0.434,0.570,0.704)
```

Part III – Calibration and determination. The following results were obtained when each of a series of standard silver solutions was analysed by flame atomic-absorption spectrometry.

Concentration, ng/ml	Absorbance
10	0.251
15	0.390
20	0.498
25	0.625
30	0.763
0	0.003
5	0.127

Task 1 *Determine the slope and intercept of the calibration plot, and their confidence limits.*

```
Conc = c(10,15,20,25,30,0,5)
Abs2 = c(0.251,0.390,0.498,0.625,0.763,0.003,0.127)

# hint: fit a regression model
# Call it something like "RegModel" or "myNewModel2"
# use the commands summary(), coef() and confint()
```

Part IV – The method of standard additions The gold content of a concentrated sea-water sample was determined by using atomic-absorption spectrometry with the method of standard additions. The results obtained were as follows:

Gold added, ng per ml of concentrated sample	Absorbance
30	0.413
40	0.468
50	0.528
60	0.574
70	0.635
0	0.257
10	0.314
20	0.364

Determine the estimates for the slope and intercept. Additionally comment on the associated p-values from the summary output.

```
Gold = c(30,40,50,60,70,0,10,20)
Absrb= c(0.413,0.468,0.528,0.574,0.635,0.257,0.314,0.364)

lm(Absrb ~ Gold)
summary(lm(Absrb ~ Gold))

# look at summary output for asterisk signs
```

Part V – Comparing analytical methods An ion-selective electrode (ISE) determination of sulphide from sulphate-reducing bacteria was compared with a gravimetric determination. The result, obtained were expressed in milligrams of sulphide.

```
Sulphide (ISE method): 108,12,152,3,106,11,128,12,160,128
Sulphide (gravimetry): 105,16,113,0,108,11,141,11,182,118
```

Compute the simple linear regression equation for the case where

1) The ISE method is the independent variable,
2) The ISE method is the dependent variable.

Write down the regression equations for both models.

Which approach (if any) is more suitable?