

## 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

	Concentration, ng/ml	Absorbance
	10	0.251
	15	0.390
spectrometry.	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 concen- trated 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 results, 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?