Absorbtivities $\varepsilon_{\lambda 1}$, $\varepsilon_{\lambda 2}$, $\varepsilon_{\lambda 3}$, $\varepsilon_{\lambda 4}$ are determined from calibration curves.
$A_{\lambda 1}$, $A_{\lambda 2}$, $A_{\lambda 3}$, $A_{\lambda 4}$ are measured.
[Cu] and [Nd] are concentrations of the Cu and Nd in the unknown solution
b=1cm

$$A_{\lambda 1} = \varepsilon_{\lambda 1,Cu} b[Cu] + \varepsilon_{\lambda 1,Nd} b[Nd] + error$$
$$A_{\lambda 2} = \varepsilon_{\lambda 2,Cu} b[Cu] + \varepsilon_{\lambda 2,Nd} b[Nd] + error$$
$$A_{\lambda 3} = \varepsilon_{\lambda 3,Cu} b[Cu] + \varepsilon_{\lambda 3,Nd} b[Nd] + error$$
$$A_{\lambda 4} = \varepsilon_{\lambda 4,Cu} b[Cu] + \varepsilon_{\lambda 4,Nd} b[Nd] + error$$

it can be shown that putting the derivatives of SS equal zero results in the following matrix (*minus* the **error** term):

$$\begin{pmatrix} A_{\lambda 1} \\ A_{\lambda 2} \\ A_{\lambda 3} \\ A_{\lambda 4} \end{pmatrix} = \begin{pmatrix} \varepsilon_{\lambda 1,Cu} & \varepsilon_{\lambda 1,Nd} \\ \varepsilon_{\lambda 2,Cu} & \varepsilon_{\lambda 2,Nd} \\ \varepsilon_{\lambda 3,Cu} & \varepsilon_{\lambda 3,Nd} \\ \varepsilon_{\lambda 4,Cu} & \varepsilon_{\lambda 4,Nd} \end{pmatrix} \begin{pmatrix} [Cu] \\ [Nd] \end{pmatrix}$$

$A = \varepsilon \cdot C$
The only unknown is matrix C which contains the parameters (concentrations) we wish to estimate: [Cu] and [Nd].
The **A** and ε matrices are known. Solving for C now requires matrix algebra:

$$(\varepsilon^T \varepsilon)^{-1} \varepsilon^T A = C$$

The LINEST function in Excel is the easiest way of doing regression:

The LINEST function in Excel is the easiest way of doing regression:

X-range: Make two columns with the independent variables (one column with ε[Cu] values at the 4 wavelengths and one column with the ε[Nd] values at the 4 different wavelengths)

Y range: Make a column with the measured dependent variable (Absorbance of the unknown mixture at the 4 wavelengths)

Select a range of 5x3 cells and type:

LINEST(Y-range, X-range, 1, 1) then Ctrl+Shift+Enter (LINEST is an *array* function. Such functions need to be activated using Ctrl+Shift+Enter).

Linest gives the following numbers: (see page 31 in your lab manual)

slope2	slope1	intercept
s_e of slope2	s_e of slope1	s_e of intercept
R^2	RMSE	
F	df	
SS(reg)	SS(resid)	

Note: the parameters run from right to left,
i.e. if the X range lists the ε_{Cu} in the first column,
Then the [Cu] will be the second column (slope 1) in the Linest output:

Example Excel:

	A	B	C	D
1	λ (nm)	εNd	εCu	A
2				
3	523	0.01	0.0285	0.0551
4	577	5.703	0.0602	0.1359
5	660	5.9	3.14	0.0861
6	743	5.703	9.68	0.4024

Using: LINEST(D3:D6,B3:C6,1,1):

0.0312065	0.00277835	0.05713867
0.0155653	0.02454436	0.10867783
0.84381957	0.10852718	#N/A
2.7014254	1	#N/A
0.06363558	0.01177815	#N/A

Since ε_{Nd} listed in the first of the two X columns, the [Nd] is the second column in Linest:

NOTE: I just used absorptivity values from a previous student report. Not sure about the quality of the data. In this specific example, the results are:
[Cu] = 0.03 (0.02)M
and [Nd] = 0.00_3(0.02) M (basically zero [Nd] since error is larger than the concentration)