

# Matlab Code

```
1 %% PLS algorithm for diethyl carbonate and ethanol
2 clear all ; close all
3 load ('Pascal.mat') % calibration data - spectra of the standard mixtures
4 wn= StdSpectra (1:1866,1) ; % wave number
5 abs = transpose ( StdSpectra (1:1866,2:73) ); % = matrix X, absorbance
6 conz = Standards (1:72,1:2:3) ; % = matrix Y, weight percentages of the standard mixtures
7 % conz =[ DEC | H2O| EtOH ]
8
9 %% Plot of the infrared spectra
10 figure ()
11 set (gcf, 'Renderer', 'Painters');
12 plot (wn , abs (1:72,1:1866) )
13 axis ([400 4000 0 1.5])
14 set (gca, 'FontSize',14);
15 xlabel ('wave number [cm ^{-1}]', FontSize =14)
16 ylabel ('absorbance', FontSize =14)
17
18 %% PrePLS - Finding the optimum number of PLS - components
19 [XL,YL,XS,YS,BETA, PCTVAR,MSE, stats] = plsregress (abs,conz,12, 'cv',10);
20
21 %% MSE
22 figure
23 plot (0:12, MSE (2,:), 'k-o')
24 axis ([0 12 0 50])
25 set (gca, 'FontSize',14);
26 ylabel ('MSE', FontSize =14)
27 xlabel ('number of PLS - components', FontSize =14)
28
29 %% PLS with optimal number of PLS - components
30 [~,~,~,~, BETAr, PCTVARr,MSER, statsr] = plsregress (abs,conz,3, 'cv',10);
31 conzfit = [ ones (size (abs,1),1) abs ]* BETAr ;
32
33 %R^2
34 TSS = sum (( conz - mean ( conz ) ).^2) ;
35 RSS = sum (( conz - conzfit ).^2) ;
36 Rsquared = 1 - RSS ./ TSS
37
38 % Residual plot
39 stem ( statsr.Yresiduals (:,1), 'ko')
40 hold on
41 stem ( statsr.Yresiduals (:,2), 'ro')
42 hold off
43 set (gca, 'FontSize',14);
44 axis ([0 72 -3 3])
45 xlabel ('number of standard mixture', FontSize =16) ;
46 ylabel ('weight percent - residuals', FontSize =16) ;
47 legend ('diethyl carbonate','ethanol', FontSize =16)
48
49 % standard error
50 Bias = mean ( statsr.Yresiduals );
51 n= numel ( statsr.Yresiduals );
52 SE= sqrt ( sum (( statsr.Yresiduals - Bias ).^2) /(n -1) )
53
54 % correlation
55 conzfitr = [ ones (size (abs,1),1) abs ]* BETAr ;
56 plot ( conz (:,1),conzfitr (:,1), 'ko')
57 hold on
58 plot ( conz (:,2),conzfitr (:,2), 'ro')
59 hold off
60 set (gca, 'FontSize',14);
61 xlabel ('weight percent - standard mixture', FontSize =16) ;
62 ylabel ('weight percent - model', FontSize =16) ;
63 legend ('diethyl carbonate','ethanol', FontSize =16)
64
65 %% sample evaluation
66 load ('Samples.mat') % sample measurement data - spectra of the sample
67 abssample = transpose ( Samples ); % absorbance of the unknown sample
68 conzsampl = [ ones (size (abssample,1),1) abssample ]* BETAr % weight percent of sample
```