

Data Preparation

```
% Extracting data for each sample
sample_data = zeros(26, 176); % Placeholder for sample data
std_avg = zeros(26, 176);      % Placeholder for average standard
deviations
conc_avg = zeros(26, 3);       % Placeholder for average concentrations
for i = 1:26
    start_index = 5 * (i - 1) + 1;
    end_index = start_index + 4;
    sample_data(i, :) = DATA(start_index:end_index, :);
    std_avg(i, :) = mean(std(DATA(start_index:end_index, :)), 1) / sqrt(5);
    conc_avg(i, :) = mean(CONC(start_index:end_index, :), 1);
end
disp('The sample data is: ');
```

The sample data is:

```
disp(sample_data);
```

0.1302	0.3089	0.1039	0.1189	0.0578	-0.0478	0.1588	-0.0006	0.1620	0.0463	0
0.2032	-0.0730	0.1673	-0.0523	0.0353	-0.0662	-0.0078	0.2933	-0.0777	0.2210	-0
0.0346	0.2002	0.1761	0.0077	0.3967	0.0596	0.0782	0.0446	0.0968	0.3388	0
0.0523	0.2343	0.2731	-0.1385	0.3130	-0.0480	-0.0383	0.0395	0.2535	0.1996	0
-0.2183	0.4733	-0.0739	-0.0374	0.1803	-0.1497	0.0794	0.4352	-0.1224	0.2719	-0
0.1283	0.2529	0.2518	0.3878	0.4398	0.0094	-0.1839	0.3480	0.0573	0.3670	0
0.1733	0.1568	0.0067	0.0830	0.1689	-0.0763	0.1984	0.2156	-0.3749	0.1861	0
0.1065	0.3416	0.1527	0.2373	-0.0584	-0.1165	-0.1427	0.1993	0.1678	0.0815	-0
-0.0278	0.0969	0.1125	0.3269	0.0480	-0.0581	0.5591	0.1896	0.0407	-0.0278	0
0.4414	-0.0396	0.0724	0.1643	0.1500	0.1652	0.1145	-0.0433	0.1374	0.1968	0
0.0237	0.3938	-0.0588	-0.0284	0.0348	0.0559	0.2587	-0.0289	0.1766	0.1381	0
0.0885	0.0263	0.2705	0.2648	0.1085	0.1446	0.0589	0.0840	0.3473	0.2093	0
0.0327	0.1405	-0.0990	0.1668	-0.0061	-0.0971	0.0576	0.0075	0.0574	0.2090	0
0.1391	0.1541	0.1769	-0.1248	0.0221	0.0422	-0.0814	0.3133	-0.0202	0.4556	0
0.1646	0.0340	0.1032	0.2148	0.2566	-0.0862	0.3806	-0.3065	0.0978	0.2560	0
0.1503	0.2376	0.0764	0.3233	0.1736	0.1323	0.3933	0.0822	0.0928	0.2496	0
-0.0551	0.2199	0.1827	0.2572	0.0606	-0.1004	0.0614	0.5740	-0.0726	0.1763	0
0.0667	0.2581	-0.0799	0.1407	0.1975	0.0578	0.1797	0.0623	0.3247	0.2390	0
-0.1508	0.6758	-0.1155	0.0240	0.0762	0.2312	-0.0076	0.1317	-0.0141	0.2316	0
0.1671	0.1964	0.4252	0.0130	0.1084	0.3530	0.3977	0.3359	0.2152	0.1149	0
0.0186	0.0714	0.1489	0.1792	0.1475	-0.2490	0.1875	0.0347	0.1763	0.1988	0
0.3957	-0.1788	0.2215	0.1248	0.1307	0.0143	0.3645	-0.1681	0.2657	-0.1090	0
-0.0344	0.3727	0.2039	0.0304	0.2901	-0.0398	-0.0592	0.4047	0.2215	0.2095	0
-0.0485	-0.0358	0.2135	-0.1266	-0.0977	-0.0559	0.2776	0.0537	0.0631	-0.0080	-0
0.0983	0.2153	-0.1923	0.1739	-0.1932	0.0868	0.1204	0.2272	-0.0140	0.1839	0
-0.0495	0.0181	0.2911	0.2088	0.4197	0.0069	0.4593	0.1634	0.0348	0.2891	0

```
disp('Average concentration data is: ');
```

Average concentration data is:

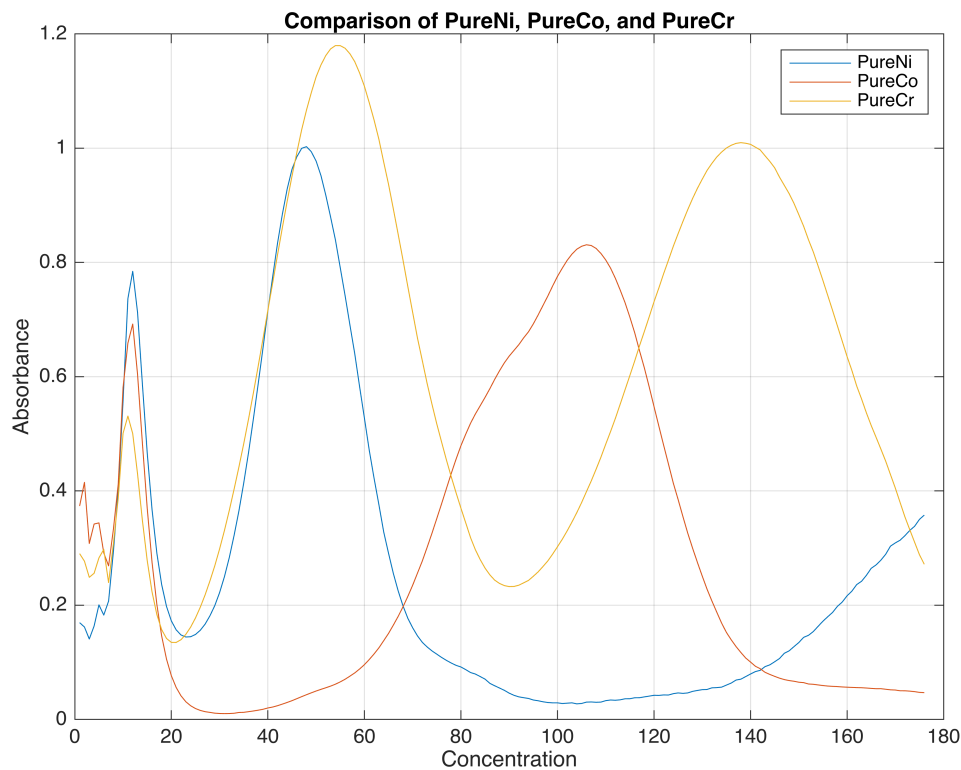
```
disp(conc_avg);
```

0.0031	0.0157	0.0069
0.0031	0.0157	0.0206
0.0031	0.0157	0.0344
0.0031	0.0471	0.0069
0.0031	0.0471	0.0206
0.0031	0.0471	0.0344

0.0031	0.0786	0.0069
0.0031	0.0786	0.0206
0.0031	0.0786	0.0344
0.0092	0.0157	0.0069
0.0092	0.0157	0.0206
0.0092	0.0157	0.0344
0.0092	0.0471	0.0069
0.0092	0.0471	0.0206
0.0092	0.0471	0.0344
0.0092	0.0786	0.0069
0.0092	0.0786	0.0206
0.0092	0.0786	0.0344
0.0153	0.0157	0.0069
0.0153	0.0157	0.0206
0.0153	0.0157	0.0344
0.0153	0.0471	0.0069
0.0153	0.0471	0.0206
0.0153	0.0471	0.0344
0.0153	0.0786	0.0069
0.0153	0.0786	0.0344

Part A: Visualization and Multilinear Regression

```
% Visualization
figure();
set(gcf, 'Name', 'Comparison of PureNi, PureCo, and PureCr');
plot(PureNi);
hold on;
plot(PureCo);
plot(PureCr);
hold off;
legend('PureNi', 'PureCo', 'PureCr');
xlabel('Concentration');
ylabel('Absorbance');
title('Comparison of PureNi, PureCo, and PureCr');
grid on;
```



```
% Index and data for multilinear regression
```

```
[maxValue_Ni, maxIndex_Ni] = max(PureNi);
```

```
[maxValue_Cr, maxIndex_Cr] = max(PureCr);
```

```
[maxValue_Co, maxIndex_Co] = max(PureCo);
```

```
Y_sample_MLR = [sample_data(:, maxIndex_Ni), sample_data(:, maxIndex_Cr),  
sample_data(:, maxIndex_Co)];
```

```
% Multilinear regression
```

```
B_sample_MLR = inv(Y_sample_MLR' * Y_sample_MLR) * Y_sample_MLR' * conc_avg;
```

```
RMSE_sample_MLR = norm(conc_avg - Y_sample_MLR * B_sample_MLR);
```

```
% RMSE by Leave-One-Out Cross-Validation for OLS
```

```
RMSE_LOOCV_OLS = LOOCV_OLS(Y_sample_MLR, conc_avg);
```

```
disp('RMSE by LOOCV for OLS: ');
```

```
RMSE by LOOCV for OLS:
```

```
disp(RMSE_LOOCV_OLS);
```

```
0.0007    0.0453    0.0171
```

Part B: Partial Least Squares Regression (PLSR)

```
num_PCs = 10;
```

```
RMSE_PCR = zeros(num_PCs, 3);
```

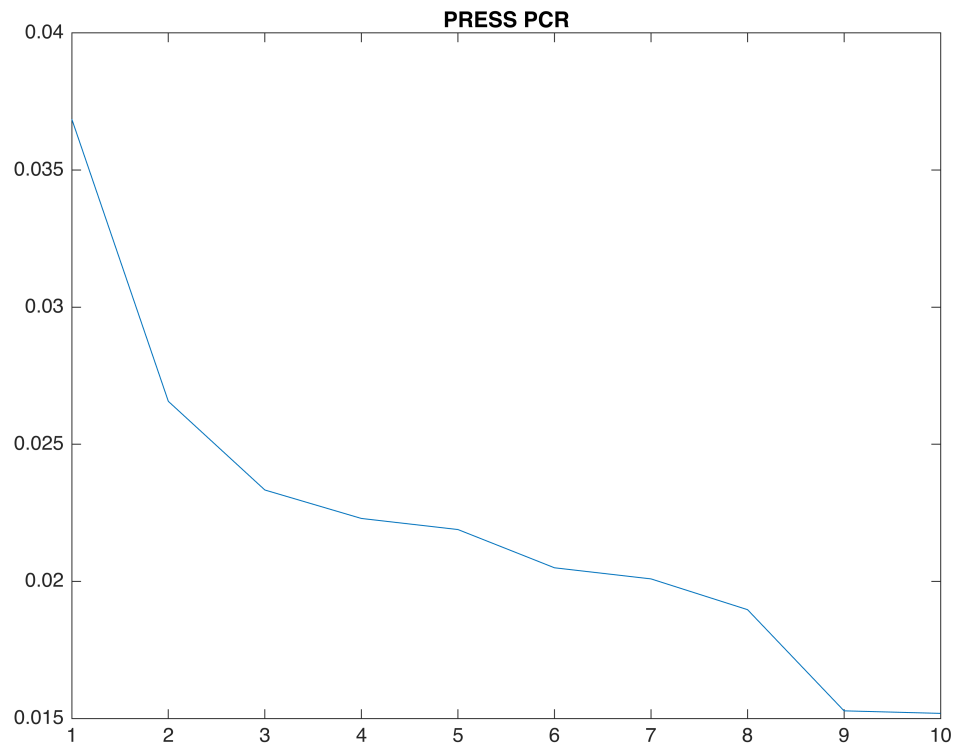
```
for i = 1:num_PCs
```

```
    RMSE_PCR(i, :) = LOOCV_PCR(sample_data, conc_avg, i);
```

```
end
```

```
PRESS_PCR = sum(RMSE_PCR, 2);
```

```
figure();
set(gcf, 'Name', 'PRESS PCR');
plot(PRESS_PCR);
title('PRESS PCR');
```



```
disp('RMSE by L00CV for PCR: ');
```

RMSE by L00CV for PCR:

```
disp(RMSE_PCR);
```

0.0037	0.0212	0.0119
0.0037	0.0143	0.0086
0.0030	0.0126	0.0078
0.0029	0.0118	0.0076
0.0028	0.0114	0.0077
0.0026	0.0107	0.0072
0.0025	0.0103	0.0072
0.0024	0.0099	0.0067
0.0019	0.0081	0.0053
0.0018	0.0081	0.0053

```
disp('PRESS by L00CV for PCR: ');
```

PRESS by L00CV for PCR:

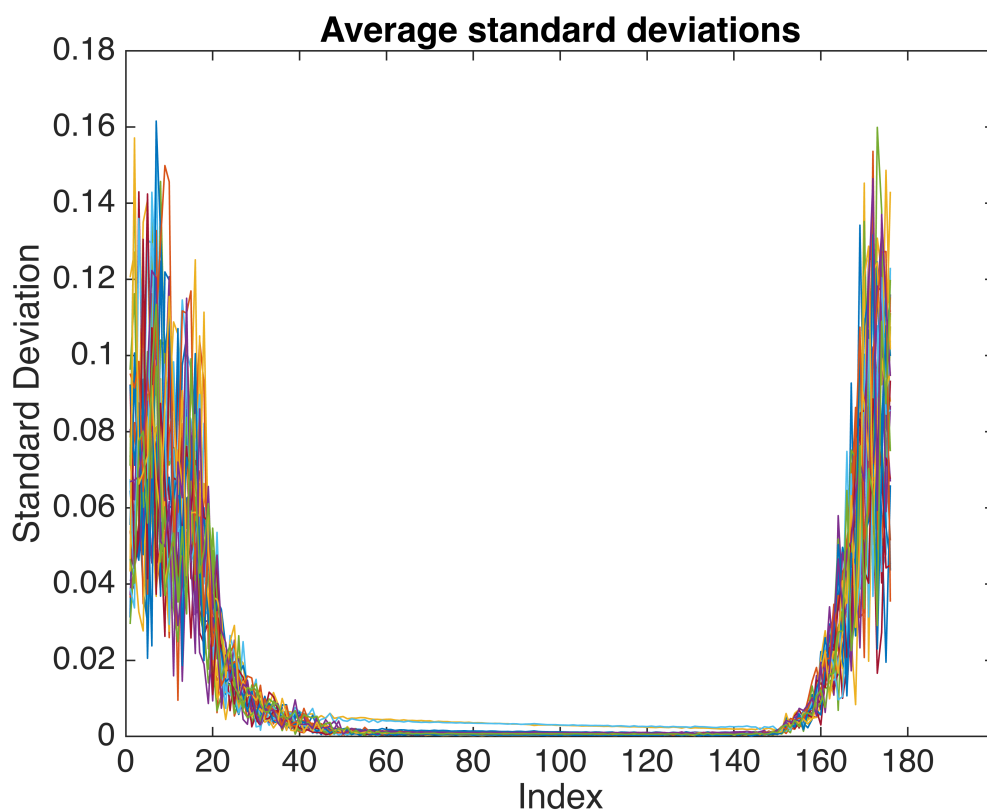
```
disp(PRESS_PCR);
```

```
0.0369
0.0266
0.0233
```

```
0.0223
0.0219
0.0205
0.0201
0.0190
0.0153
0.0152
```

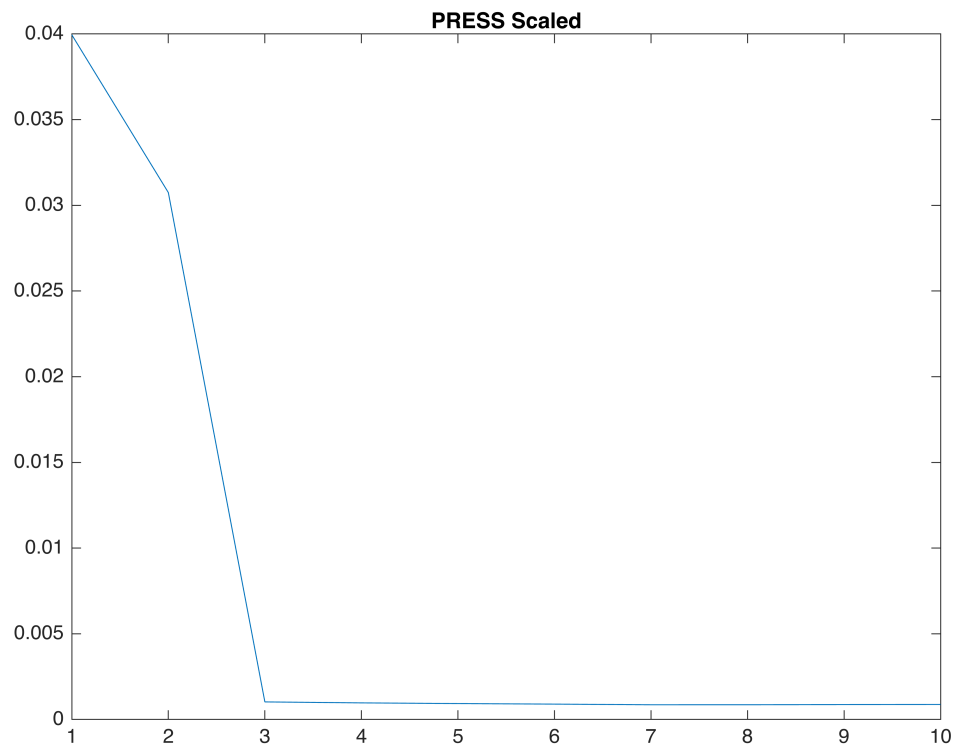
Part C: Scaled PLSR (SPCR)

```
figure();
set(gcf, 'Name', 'Average standard deviations');
plot(std_avg');
title('Average standard deviations');
ylabel('Standard Deviation');
xlabel('Index');
```



```
stds = mean(std_avg); % Assuming variation only along wavelength not
mixture
L = diag(stds);
Y_scaled = sample_data * inv(L); % Scaling
RMSE_SPCR = zeros(num_PCs, 3);
for i = 1:num_PCs
    RMSE_SPCR(i, :) = L00CV_PCR(Y_scaled, conc_avg, i);
end
PRESS_Scaled = sum(RMSE_SPCR, 2);
figure();
```

```
set(gcf, 'Name', 'PRESS Scaled');
plot(PRESS_Scaled);
title('PRESS Scaled');
```



```
disp('RMSE by L00CV for SPCR: ');
```

RMSE by L00CV for SPCR:

```
disp(RMSE_SPCR);
```

0.0031	0.0260	0.0108
0.0033	0.0212	0.0063
0.0001	0.0005	0.0004
0.0001	0.0005	0.0004
0.0001	0.0005	0.0004
0.0001	0.0005	0.0003
0.0001	0.0004	0.0003
0.0001	0.0004	0.0003
0.0001	0.0005	0.0003
0.0001	0.0005	0.0003

```
disp('PRESS by L00CV for SPCR: ');
```

PRESS by L00CV for SPCR:

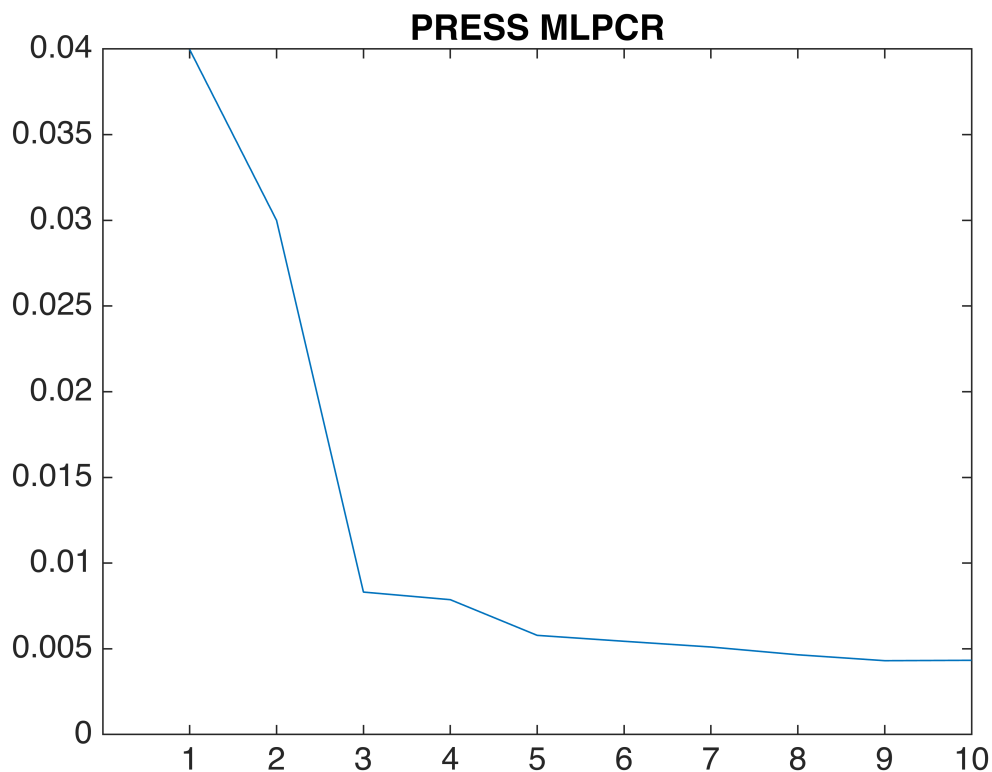
```
disp(PRESS_Scaled);
```

0.0400
0.0307
0.0010
0.0010

```
0.0009
0.0009
0.0009
0.0009
0.0009
0.0009
```

Part D: MLPCA

```
RMSE_MLPCR = zeros(num_PCs, 3);
for nPC = 1:num_PCs
    RMSE_MLPCR(nPC, :) = L00CV_MLPCR(sample_data, conc_avg, std_avg, nPC);
end
PRESS_MLPCR = sum(RMSE_MLPCR, 2);
figure();
set(gcf, 'Name', 'PRESS MLPCR');
plot(PRESS_MLPCR);
title('PRESS MLPCR');
```



```
disp('RMSE by L00CV for MLPCR: ');
```

RMSE by L00CV for MLPCR:

```
disp(RMSE_MLPCR);
```

```
0.0033    0.0252    0.0114
0.0032    0.0182    0.0086
0.0004    0.0069    0.0010
```

0.0004	0.0064	0.0011
0.0004	0.0044	0.0011
0.0004	0.0041	0.0010
0.0004	0.0038	0.0009
0.0003	0.0034	0.0009
0.0003	0.0031	0.0008
0.0003	0.0032	0.0008

```
disp('PRESS by L00CV for MLPCR: ');
```

PRESS by L00CV for MLPCR:

```
disp(PRESS_MLPCR);
```

0.0400
0.0300
0.0083
0.0079
0.0058
0.0054
0.0051
0.0047
0.0043
0.0043