Challenge. Chimiometrie XIX, Paris 2018

Locally Weighted Regression

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1. Clean up calibration set

- There are 207 redundant samples in the calibration set.
- There are 54 spectra in validation set that have identical match in the calibration set.

2. Pre-process calibration and validation sets

- Savitsky-Golay derivative (1,15,2) and SNV was found to give the best results.

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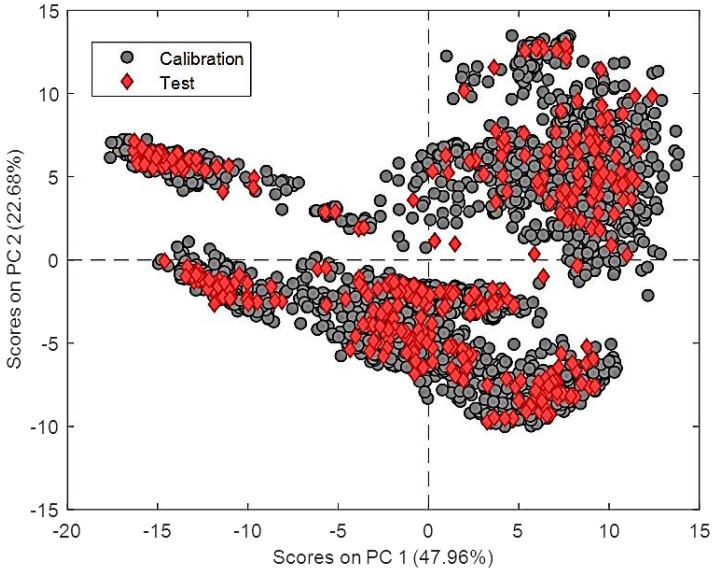
3. Calculate distances

- Un-scaled mahalanobis distances in the PCA score space (10 factors) of calibration spectra were used.

- Distance from each sample in validation set was calculated to the nearest samples in the score space and nn=150 (local) samples were found to be optimal and were indexed for each validation sample.



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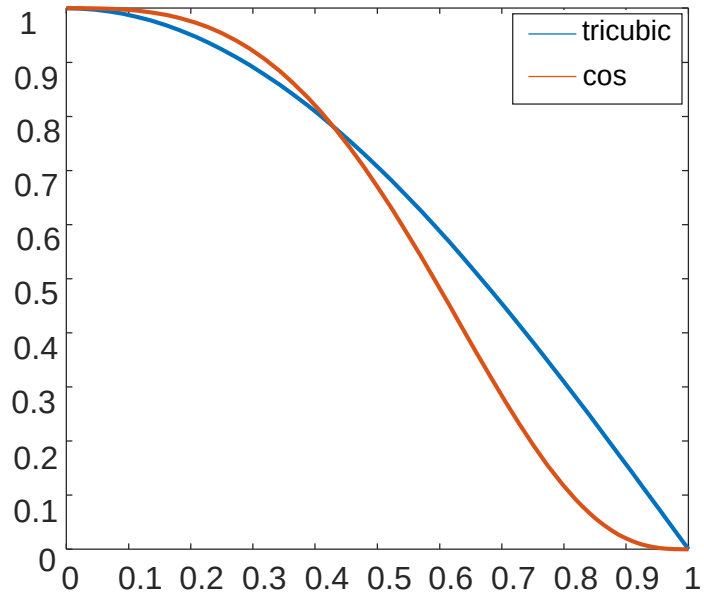
4. Remove extreme Y values

- A Global PLS was applied.
- Samples with extreme reference values with respect to the estimated values (*y_est*) were removed.
- A wide window (> *y_est* - 30 & <*y_est* + 30) was used for pruning.

5. Apply a weight function to local samples

- A cosine weighting function (w) was used instead of the traditional tri-cubic function in order to weight the local samples in proportion to their scaled distances (d):

$$w = \cos\left(\frac{\pi}{2}d\right);\ |d| < 1$$



6. PLS regression on local samples

- A PLS regression (11 factors) was performed on weighted local samples to predict each validation sample.

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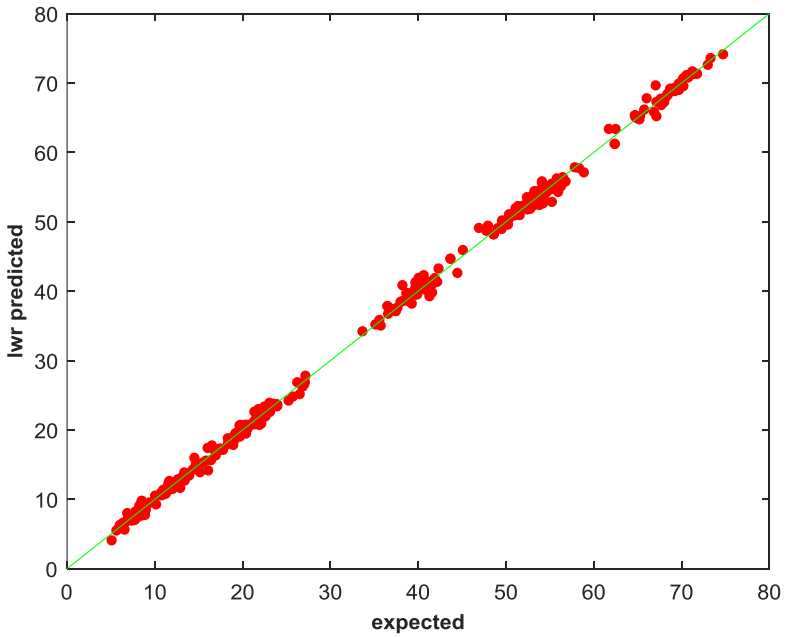
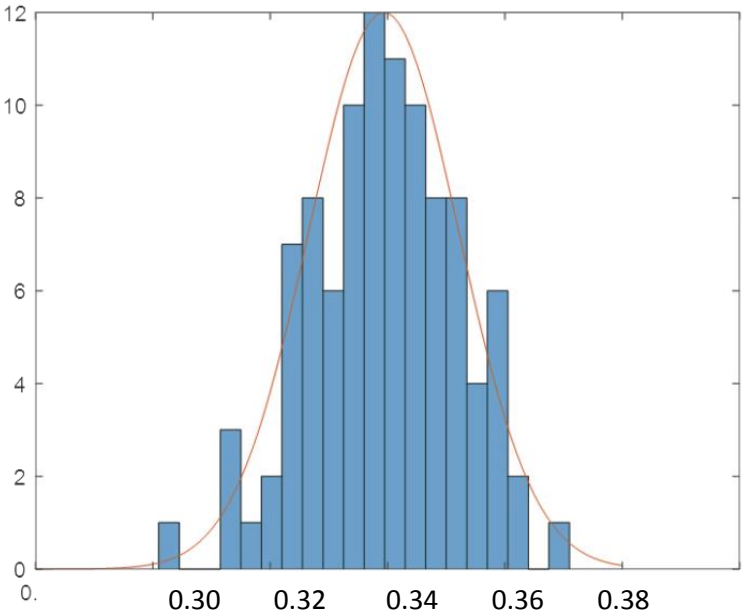
Results

MAD=0.32





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Thank you

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