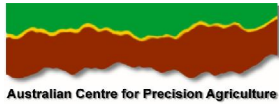


# ParLeS v2.0 freeware to pre-process spectra and perform Partial Least Squares Regression (PLSR) with leave-one-out cross validation



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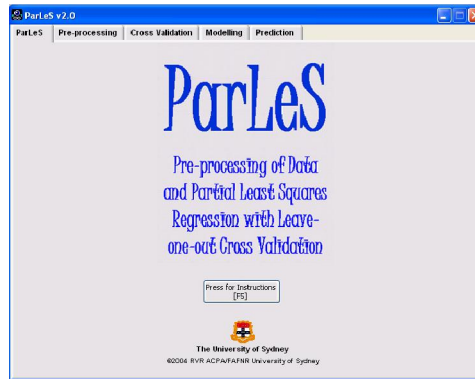
[www.usyd.edu.au/su/agric/acpa/people/rvrossel/soft01.htm](http://www.usyd.edu.au/su/agric/acpa/people/rvrossel/soft01.htm)  
 e-mail: [r.rossel@agec.usyd.edu.au](mailto:r.rossel@agec.usyd.edu.au)

PLSR is a popular modelling technique in chemometrics, commonly used for quantitative analysis

PLSR is used to construct predictive models when there are many factors that are highly collinear, e.g. in spectroscopy.

PLSR will try to find a few PLS factors that explain most of the variation in both predictors X and response y

PLSR maximises the covariance between the X and y scores

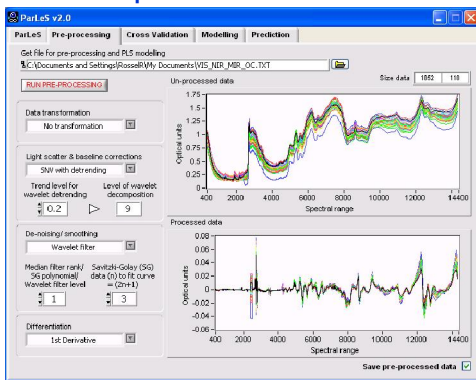


The emphasis of PLSR is on predicting the response.

However, when used interactively with proper validation and graphics PLSR provides a good causal insight into the underlying relationships between the spectra and response variables.

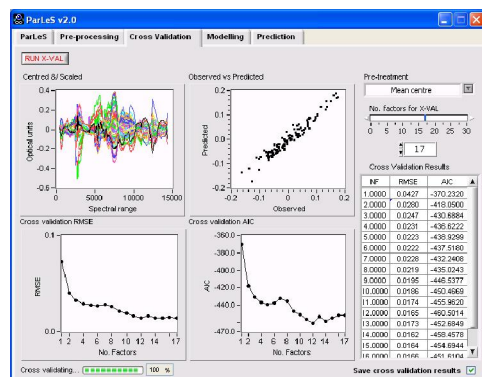
Algorithm described in Martens & Næs (1989)

## 1. Pre-process data



(i.) Data transformations, (ii.) MSC, SNV, wavelet de-trending (iii) median filter, Savitzki-Golay, wavelet de-noising, and (iv) 1<sup>st</sup> and 2<sup>nd</sup> derivatives

## 2. LOO-X-validation



(i) Mean centre &/ variance scaling, (ii) leave-one-out cross validation to determine optimal number of factors for PLS regression modelling

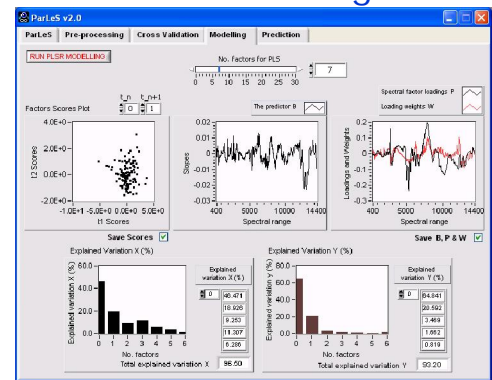
ParLeS v2.0 performs the following tasks:

- i. pre-processing
- ii. mean centering &/ or variance scaling
- iii. leave-one-out cross validation
- iv. PLSR modelling
- v. PLSR predictions

The following data may be saved for external plotting and analysis:

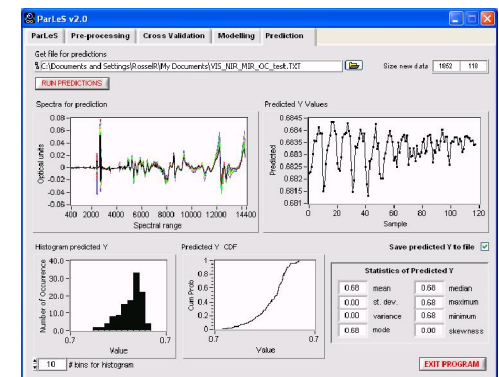
- i. pre-processed spectra,
- ii. cross validation predictions and their statistics,
- iii. PLSR scores (t), loadings (P), weights (W) slopes (B) and
- iv. predictions

## 3. PLSR modelling



PLSR modelling showing factor scores (t), loadings weights (W), chemical loadings (P), slopes of regression (B) and % variation in X and y

## 4. Predict unknowns



Predictions of unknowns using selected number of factors (in 3. above) and with new X. Predictions and their statistics shown

## References

1. Martens H., Næs, T. (1989). Multivariate Calibration. John Wiley & Sons, Chichester
2. Viscarra Rossel R.A. 2005. ParLeS v2.0 freeware to pre-process spectra & perform PLSR with leave-one-out cross validation. [www.usyd.edu.au/su/agric/acpa/people/rvrossel/soft01.htm](http://www.usyd.edu.au/su/agric/acpa/people/rvrossel/soft01.htm)