

Competitive Adaptive Reweighted Sampling *coupled with Partial Least Squares Regression* (CARS)

Version 2.0

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Platform

The current version is coded and tested in MATLAB 7.6.0 in Window Operating Systems. If any questions about running this software, please feel free to contact us.

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1 Main functions

ID	File	Descriptions
1	<i>pls.m</i>	Main program for building a PLSR model.
2	<i>plsval.m</i>	Make predictions using PLSR model
3	<i>plscvfold.m</i>	K-fold cross validation for choosing the number of latent variables
4	<i>plsmccv.m</i>	Monte Carlo Cross Validation for choosing the number of latent variables
5	<i>Plsrdcv.m</i>	Repeated Double Cross Validation
6	<i>carspls.m</i>	Using CARS to conduct variable selection
7	<i>plotcars.m</i>	Plot the results obtained from carspls.m
8	<i>scarspls.m</i>	Simplified version of CARS: SCARS

2 Datasets

Corn_mp51.mat: www.eigenvector.com. This is the corn NIR data measured on mp5 instrument with moisture as the response.

3 Usage:

Please type **help filename** in the MATLAB prompt window for detailed information. For example:

```
>> help carspls
+++ CARS: Competitive Adaptive Reweighted Sampling method for variable selection.
+++ num: the number of Monte Carlo Sampling runs, default(50).
+++ method: pretreatment method.
+++ A: the maximal number of LVs to be extracted.
+++ Hongdong Li, Dec.15, 2008.
+++ Advisor: Yizeng Liang, yizeng_liang@263.net
+++ lhdcso@gmail.com
+++ Reference: Li H-D, Liang Y-Z, Xu Q-S, Cao D-S: Key wavelengths screening using
               competitive adaptive reweighted sampling method for multivariate calibration.
               Anal Chim Acta 2009, 648(1):77-84.
+++++
```

4 Example script:

Along with the software, there are two example scripts, with filename ***example_nir.m*** and ***test_package_functions.m***, which shows how to run CARS program to get the optimal combination of variables using a NIR dataset. Just run this program, and you will see how CARS works.

5 Reference:

[1] Li H-D, Liang Y-Z, Xu Q-S, Cao D-S: Key wavelengths screening using competitive adaptive reweighted sampling method for multivariate calibration. *Anal Chim Acta* 2009, 648(1):77-84.