## **RRegrs Flow**

- 1) Load parameters and dataset
  - Load Parameters from **CSV** as data frame → Param.df
  - Load dataset from **CSV** as data frame → ds
- 2) Filters not implemented
- 3) Remove near zero variance columns using RemNearOVarCols  $\rightarrow$  ds  $\rightarrow$  No0Var CSV
- 4) Scaling dataset (normalization default, standardization, etc.) using  $ScalingDS \rightarrow ds \rightarrow Scaled CSV$
- **5)** Remove correlated features using *RemCorrs* → ds
  - → Dataset without correlated features: Scaled NoCorrs CSV
  - → Correlation matrix: Scaled NoCorrs CorrMAT CSV
  - → Correlation plot before removal of features: Scaled NoCorrs Corrs PNG
  - → Correlation plot after removal of features: Scaled NoCorrs after RemCorr PNG

For each dataset SPLIT (default = 10)  $\rightarrow$  dfRes

- 6) Dataset splitting: Training and Test sets using DsSplit → ds.train, ds.test → CSVs for train and test
- 7) Feature selection not implemented but wrapper functions cold be executed
- 8) REGRESSION METHODS
- executed for each cross-validation type (non-wrapper or wrapper)
- resulted **PDF plots** for each method, split and cross-validation type
- resulted **CSV** for each method with detailed statistics
  - 8.1. Basic LM using *LMreg* → my.stats.LM appended to dfRes
  - 8.2. GLM based on AIC regression using GLMreg → my.stats.GLM appended to dfRes
  - 8.3. PLS using *PLSreg* → my.stats.PLS appended to dfRes
  - 8.4. LASSO using *LASSOreg* → my.stats.LASSO appended to dfRes
  - 8.5. RBF network with the DDA algorithm regression using RBF\_DDAreg → my.stats.rbfDDA appended to dfRes
  - 8.6. SVM radial regression using SVLMreg → my.stats.SVLM appended to dfRes
  - 8.7. SVM linear not implemented
  - 8.8. Neural Networks Regression using NNreg → my.stats.NN appended to dfRes
  - 8.9. SOM to be implemented
  - 8.10. Recursive Feature Extraction (SVM-RFE) to be implemented
  - 8.11- Other methods to be implemented

## 9) RESULTS

All statistics results (not ordered)  $\rightarrow$  df.res  $\rightarrow$  RRegrsResBySplit.csv

Averaged statistics of the results by each Regression Method & CV type

All results as data table → dt.res

Averaged results → dt.mean

Ordered averaged results → dt.mean.ord → RRegsResAvgs.csv

10) Best model selection – max adjR2.ts (+/- 0.005), min RMSE

Max adjR2.ts → Best model statistics → best.dt

adjR2.ts for the best model  $\rightarrow$  best.adjR2.ts

Add new conditions (max adjR2.ts (+/- 0.005), min RMSE)  $\rightarrow$  best.dt

Regression method for the best model → best.reg

11) Best model detailed statistics

Detailed statistics for the best model → RRegrsResBest.csv

Run the caret function with the method from the best method  $\rightarrow$  my.stats.reg

12) Y randomization for best model – default = 100 times

Using Yrandom → R2Diff.Yrand → RRegrsResBest.csv.Yrand.Hist.pdf