ROBERT v 1.0.2 2023/07/15 12:10:37
Citation: ROBERT v 1.0.2, Dalmau, D.; Alegre-Requena, J. V., 2023. https://github.com/jvalegre/robert

Command line used in ROBERT: robert --ignore [Name] --names Name --y Target_values --csv_name Robert_example.csv --csv_test Robert_example_test.csv

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CURATE

o Starting data curation with the CURATE module

o Database Robert_example.csv loaded successfully, including:
- 37 datapoints
- 11 accepted descriptors
- 1 ignored descriptors
- 0 discarded descriptors

o Analyzing categorical variables
A total of 1 categorical variables were converted using the onehot mode in the categorical option
Initial descriptors:
- x4
Generated descriptors:
- Csub-Csub
- Csub-H
- Csub-O
- H-O

o Duplication filters activated
Excluded datapoints:
- No datapoints were removed

o Correlation filter activated with these thresholds: thres_x = 0.9, thres_y = 0.001
Excluded descriptors:
- x3: R**2 = 1.0 with x1
- x1: R**2 = 0.96 with x6

o 14 columns remaining after applying duplicate and correlation filters:
- Name
- Target_values
- x2
- x5
- x6
- x7
- x8
- x9
- x10
- x11
- Csub-Csub
- Csub-H
- Csub-O

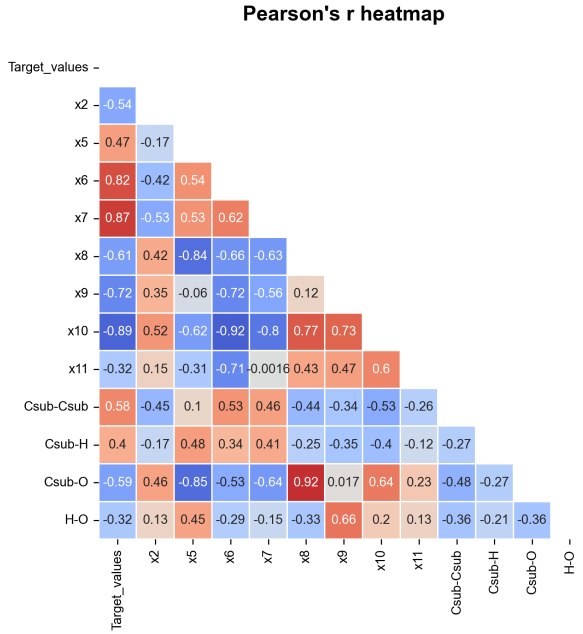
- H-O

o The Pearson heatmap was stored in CURATE/Pearson_heatmap.png.

o The curated database was stored in CURATE/Robert_example_CURATE.csv.

Time CURATE: 0.57 seconds

------- Images generated by the CURATE module -------



GENERATE

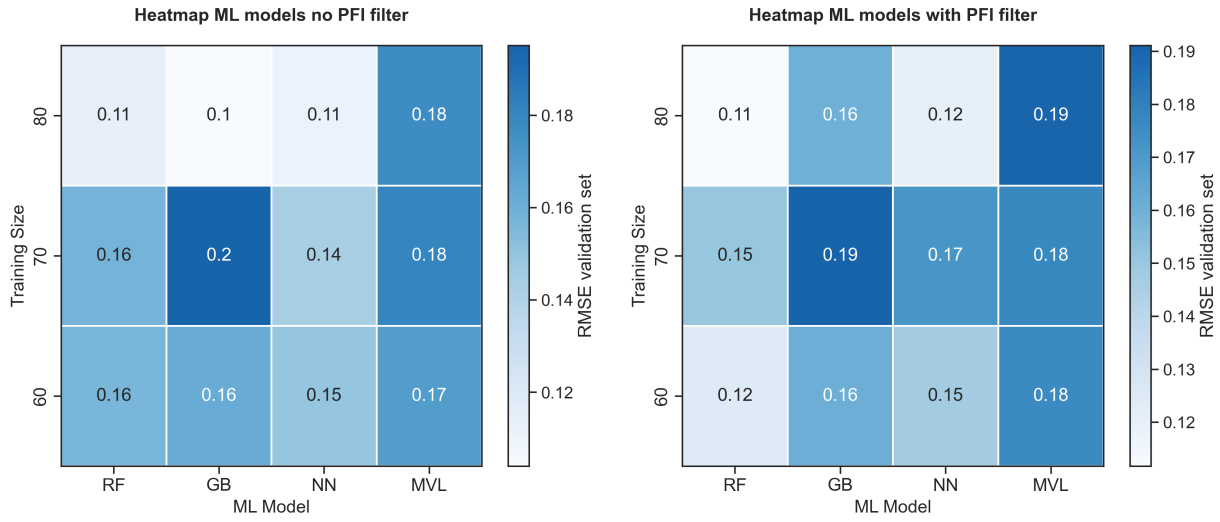
o Starting generation of ML models with the GENERATE module

o Database Robert_example_CURATE.csv loaded successfully, including:
- 37 datapoints
- 12 accepted descriptors
- 1 ignored descriptors
- 0 discarded descriptors

x WARNING! The database contains 37 datapoints, the 90% training size will be excluded (too few validation points to reach a reliable result). You can include this size using "--filter_train False".

o Starting heatmap scan with 4 ML models (['RF', 'GB', 'NN', 'MVL']) and 3 training sizes ([60, 70, 80]).
- 72 models were tested, for more information check the GENERATE_data.dat file in the GENERATE folder

------- Images generated by the GENERATE module -------



VERIFY

o Starting tests to verify the prediction ability of the ML models with the VERIFY module

------- Starting model with all variables (No PFI) -------

o ML model GB_80 (with no PFI filter) and Xy database were loaded, including:
- Target value: Target_values
- Model: GB
- Descriptors: ['x2', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10', 'x11', 'Csub-Csub', 'Csub-H', 'Csub-O', 'H-O']
- Training points: 29
- Validation points: 8

o VERIFY donut plots saved in VERIFY/VERIFY_tests_GB_80_No_PFI.png
o VERIFY test values saved in VERIFY/VERIFY_tests_GB_80_No_PFI.dat
Results of the VERIFY tests:
Original score (train set in CV): RMSE = 0.031, +- 20% threshold (thres_test option):
- 5-fold CV: NOT DETERMINED, data splitting was done with KN. CV result: RMSE = 0.22
Original score (validation set): RMSE = 0.1, +- 20% threshold (thres_test option):
o y_mean: PASSED, RMSE = 0.66 is higher than the threshold (0.12)
o y_shuffle: PASSED, RMSE = 0.8 is higher than the threshold (0.12)
o onehot: PASSED, RMSE = 0.2 is higher than the threshold (0.12)

------- Starting model with PFI filter (only important descriptors used) -------

o ML model RF_80_PFI (with PFI filter) and Xy database were loaded, including:
- Target value: Target_values
- Model: RF
- Descriptors: ['x6', 'x7', 'x9', 'x10']
- Training points: 29
- Validation points: 8

o VERIFY donut plots saved in VERIFY/VERIFY_tests_RF_80_PFI.png
o VERIFY test values saved in VERIFY/VERIFY_tests_RF_80_PFI.dat
Results of the VERIFY tests:
Original score (train set in CV): RMSE = 0.11, +- 20% threshold (thres_test option):

- 5-fold CV: NOT DETERMINED, data splitting was done with KN. CV result: RMSE = 0.22

Original score (validation set): RMSE = 0.11, +- 20% threshold (thres_test option):

o y_mean: PASSED, RMSE = 0.66 is higher than the threshold (0.13)

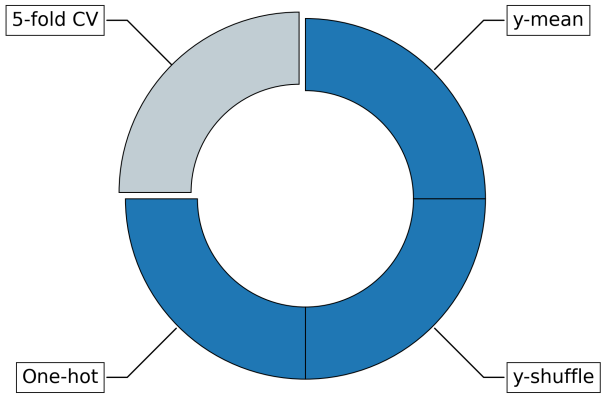
o y_shuffle: PASSED, RMSE = 0.88 is higher than the threshold (0.13)

o onehot: PASSED, RMSE = 0.21 is higher than the threshold (0.13)

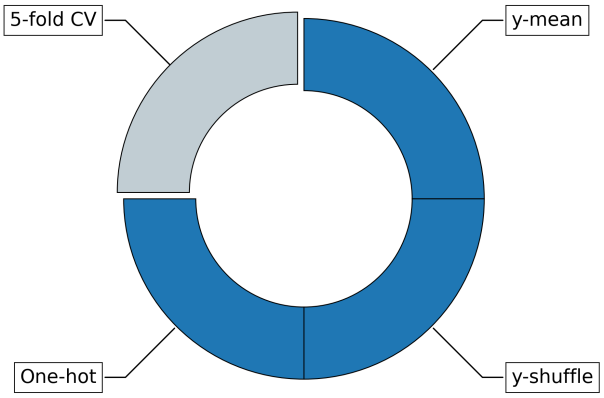
Time VERIFY: 1.95 seconds

------- Images generated by the VERIFY module -------

VERIFY tests of GB_80_No_PFI



VERIFY tests of RF_80_PFI



PREDICT

o Representation of predictions and analysis of ML models with the PREDICT module

------- Starting model with all variables (No PFI) -------

o ML model GB_80 (with no PFI filter) and Xy database were loaded, including:

- Target value: Target_values
- Model: GB
- Descriptors: ['x2', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10', 'x11', 'Csub-Csub', 'Csub-H', 'Csub-O', 'H-O']
- Training points: 29
- Validation points: 8

o Test set Robert_example_test.csv loaded successfully, including:

- 9 datapoints

x There are missing descriptors in the test set! Looking for categorical variables converted from CURATE

o The missing descriptors were successfully created

- Train set with predicted results: GB_80_train_No_PFI.csv
- Validation set with predicted results: GB_80_valid_No_PFI.csv
- Test set with predicted results: GB_80_test_No_PFI.csv

o Saving graphs and CSV databases in:

- Graph in: PREDICT/Results_GB_80_No_PFI.png

o Results saved in PREDICT/Results_GB_80_No_PFI.dat:

- Points Train:Validation:Test = 29:8:9
- Proportion Train:Validation:Test = 63:17:20
- Number of descriptors = 12
- Proportion points:descriptors = 37:12
- Train : R2 = 1.0, MAE = 0.025, RMSE = 0.031
- Validation : R2 = 0.98, MAE = 0.077, RMSE = 0.1
- Test : R2 = 1.0, MAE = 0.033, RMSE = 0.038

o SHAP plot saved in PREDICT/SHAP_GB_80_No_PFI.png
o SHAP values saved in PREDICT/SHAP_GB_80_No_PFI.dat:
- x6 = min: -0.33, max: 0.18
- x10 = min: -0.39, max: 0.17
- x5 = min: -0.1, max: 0.16
- x2 = min: -0.067, max: 0.1
- x7 = min: -0.094, max: 0.082
- x9 = min: -0.13, max: 0.051
- Csub-Csub = min: -0.056, max: 0.03
- Csub-O = min: -0.06, max: 0.019
- x11 = min: -0.043, max: 0.017
- x8 = min: -0.072, max: 0.017
- Csub-H = min: -0.019, max: 0.012
- H-O = min: 0.0, max: 0.0

o PFI plot saved in PREDICT/PFI_GB_80_No_PFI.png
o PFI values saved in PREDICT/PFI_GB_80_No_PFI.dat:
Original score (from model.score, R2) = 0.98
- x10 = 0.17 +- 0.061
- x6 = 0.12 +- 0.053
- x5 = 0.038 +- 0.029
- x7 = 0.026 +- 0.019
- x9 = 0.019 +- 0.01
- x2 = 0.017 +- 0.0096
- Csub-H = 0.0067 +- 0.0055
- x11 = 0.0054 +- 0.0058
- Csub-Csub = 0.0032 +- 0.0062
- x8 = 0.0025 +- 0.0023

o Outliers plot saved in PREDICT/Outliers_GB_80_No_PFI.png
o Outlier values saved in PREDICT/Outliers_GB_80_No_PFI.dat:
Train: 1 outliers out of 29 datapoints (3.4%)
- 21 (2.8 SDs)
Validation: 1 outliers out of 8 datapoints (12.5%)
- 22 (2.4 SDs)
Test: 0 outliers out of 9 datapoints (0.0%)

------- Starting model with PFI filter (only important descriptors used) -------

o ML model RF_80_PFI (with PFI filter) and Xy database were loaded, including:
- Target value: Target_values
- Model: RF
- Descriptors: ['x6', 'x7', 'x9', 'x10']
- Training points: 29

- Validation points: 8

o Test set Robert_example_test.csv loaded successfully, including:
- 9 datapoints
- Train set with predicted results: RF_80_train_PFI.csv
- Validation set with predicted results: RF_80_valid_PFI.csv
- Test set with predicted results: RF_80_test_PFI.csv

o Saving graphs and CSV databases in:
- Graph in: PREDICT/Results_RF_80_PFI.png

o Results saved in PREDICT/Results_RF_80_PFI.dat:
- Points Train:Validation:Test = 29:8:9
- Proportion Train:Validation:Test = 63:17:20
- Number of descriptors = 4
- Proportion points:descriptors = 37:4
- Train : R2 = 0.98, MAE = 0.076, RMSE = 0.11
- Validation : R2 = 0.97, MAE = 0.084, RMSE = 0.11
- Test : R2 = 0.99, MAE = 0.056, RMSE = 0.072

o SHAP plot saved in PREDICT/SHAP_RF_80_PFI.png
o SHAP values saved in PREDICT/SHAP_RF_80_PFI.dat:
- x6 = min: -0.38, max: 0.21
- x7 = min: -0.26, max: 0.18
- x10 = min: -0.35, max: 0.13
- x9 = min: -0.2, max: 0.062

o PFI plot saved in PREDICT/PFI_RF_80_PFI.png
o PFI values saved in PREDICT/PFI_RF_80_PFI.dat:
Original score (from model.score, R2) = 0.97
- x6 = 0.24 +- 0.11
- x7 = 0.18 +- 0.064
- x10 = 0.15 +- 0.073
- x9 = 0.047 +- 0.04

o Outliers plot saved in PREDICT/Outliers_RF_80_PFI.png
o Outlier values saved in PREDICT/Outliers_RF_80_PFI.dat:
Train: 1 outliers out of 29 datapoints (3.4%)
- 21 (4.1 SDs)
Validation: 0 outliers out of 8 datapoints (0.0%)
Test: 0 outliers out of 9 datapoints (0.0%)

Time PREDICT: 7.08 seconds

------- Images and summary generated by the PREDICT module -------

No PFI:

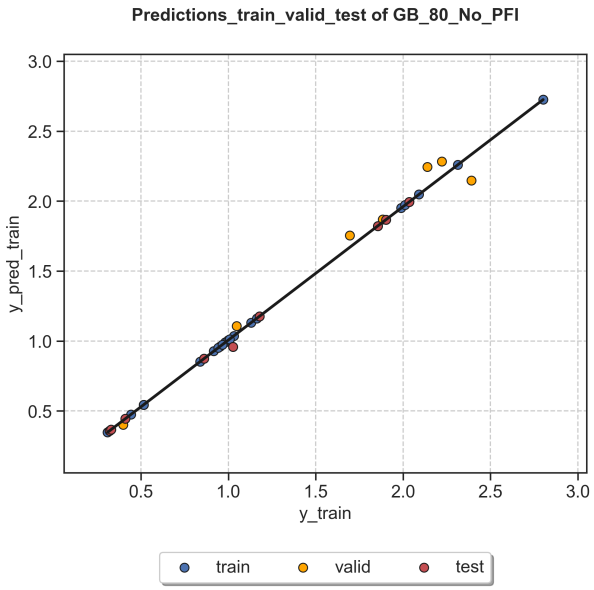
Results_GB_80_No_PFI.dat:

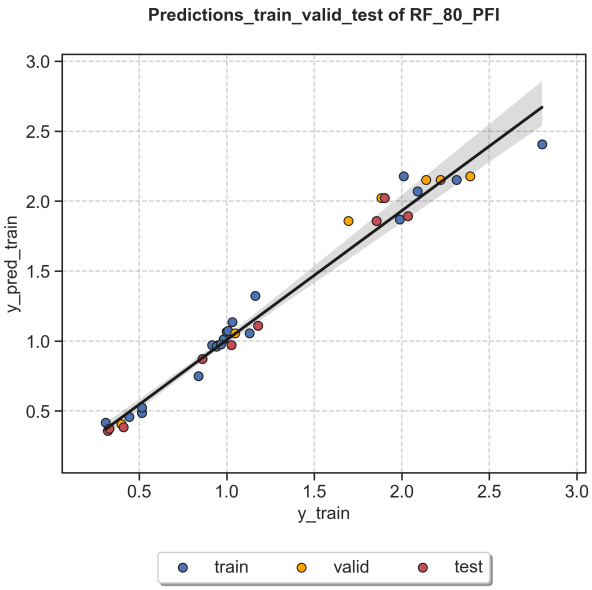
- Points Train:Validation:Test = 29:8:9
- Proportion Train:Validation:Test = 63:17:20
- Number of descriptors = 12
- Proportion points:descriptors = 37:12
- Train : R2 = 1.0, MAE = 0.025, RMSE = 0.031
- Validation : R2 = 0.98, MAE = 0.077, RMSE = 0.1
- Test : R2 = 1.0, MAE = 0.033, RMSE = 0.038

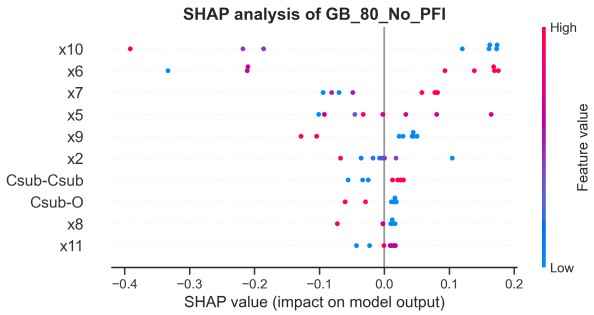
PFI:

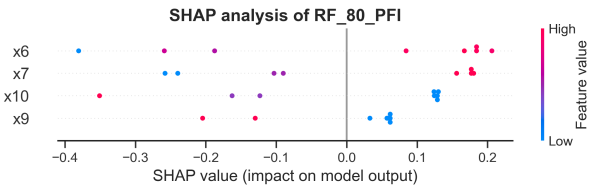
Results_RF_80_PFI.dat:

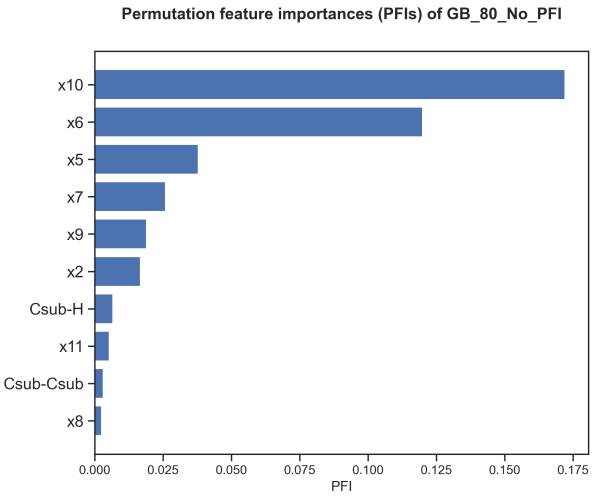
- Points Train:Validation:Test = 29:8:9
- Proportion Train:Validation:Test = 63:17:20
- Number of descriptors = 4
- Proportion points:descriptors = 37:4
- Train : R2 = 0.98, MAE = 0.076, RMSE = 0.11
- Validation : R2 = 0.97, MAE = 0.084, RMSE = 0.11
- Test : R2 = 0.99, MAE = 0.056, RMSE = 0.072

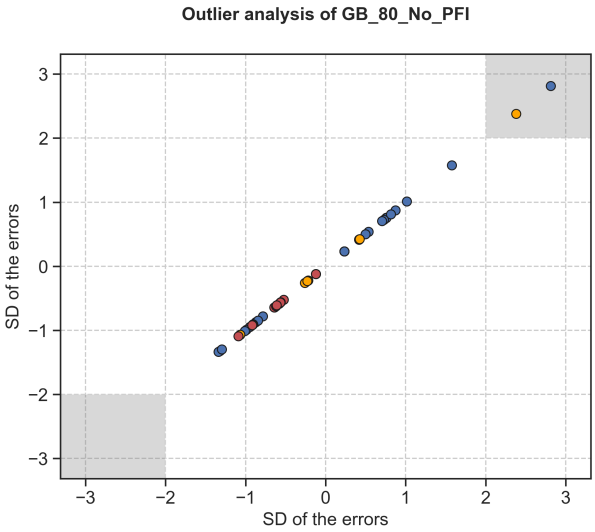


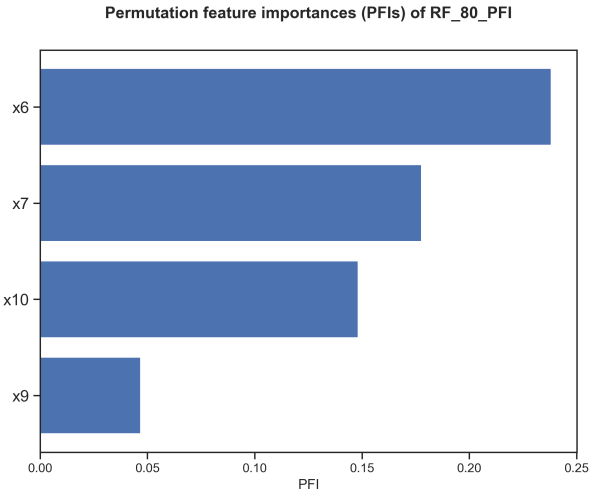


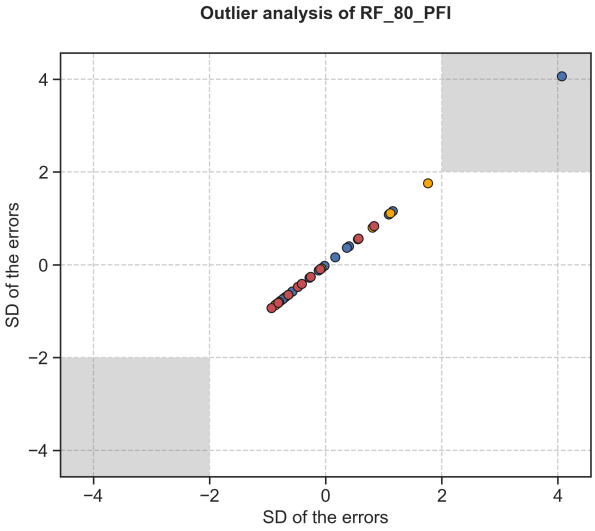





Permutation feature importances (PFIs) of GB_80_No_PFI
x10
x6
x5
x7
x9
x2
Csub-H
x11
Csub-Csub
x8
0.000
0.025
0.050
0.075
0.100
0.125
0.150
0.175
PFI


Outlier analysis of GB_80_No_PFI
SD of the errors
SD of the errors


Permutation feature importances (PFIs) of RF_80_PFI
x6
x7
x10
x9
0.00
0.05
0.10
0.15
0.20
0.25
PFI


Outlier analysis of RF_80_PFI
SD of the errors
SD of the errors