



ROBERT v 1.0.6 2024/06/28 09:47:18

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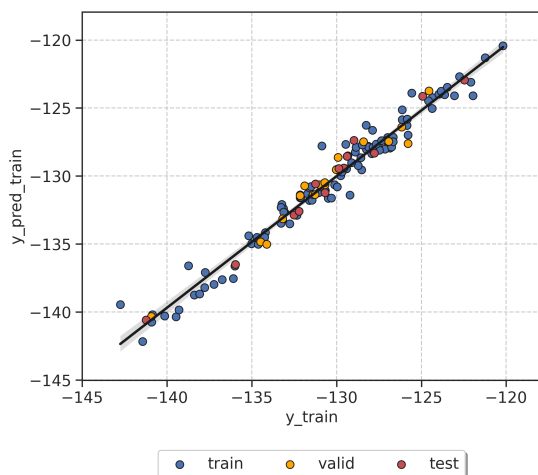
**ROBERT SCORE***This score is designed to analyze the predictive ability of the models using different metrics.***No PFI (all descriptors):**

ML model: MVL

Proportion Train:Validation:Test = 77:14:10

**STRONG****The model has a score of 10/10**

- The test set shows an  $R^2$  of 0.98
- The valid. set has 0.0% of outliers
- Using 119:8 points(train+valid.):descriptors
- The valid. set passes 4 VERIFY tests



Train :  $R^2 = 0.97$ , MAE = 0.64, RMSE = 0.89  
 Valid. :  $R^2 = 0.96$ , MAE = 0.59, RMSE = 0.76  
 Test :  $R^2 = 0.98$ , MAE = 0.61, RMSE = 0.7

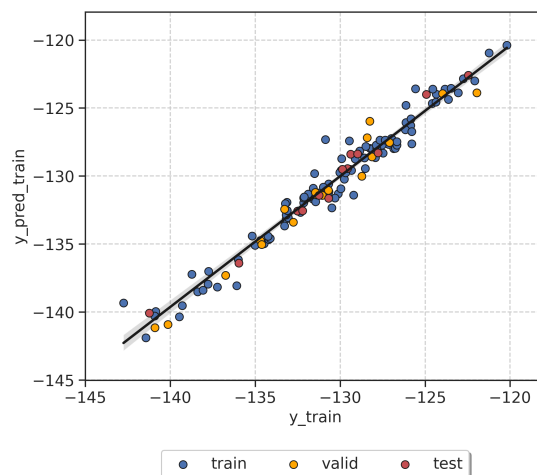
**PFI (only important descriptors):**

ML model: MVL

Proportion Train:Validation:Test = 77:14:10

**STRONG****The model has a score of 10/10**

- The test set shows an  $R^2$  of 0.98
- The valid. set has 5.6% of outliers
- Using 119:5 points(train+valid.):descriptors
- The valid. set passes 4 VERIFY tests



Train :  $R^2 = 0.96$ , MAE = 0.65, RMSE = 0.92  
 Valid. :  $R^2 = 0.97$ , MAE = 0.67, RMSE = 0.91  
 Test :  $R^2 = 0.98$ , MAE = 0.52, RMSE = 0.64

**Score thresholds** (detailed in <https://robert.readthedocs.io/en/latest/Score/score.html>) **$R^2$** 

- $R^2 > 0.85$
- $0.85 > R^2 > 0.70$
- $R^2 < 0.70$

**Outliers**

- < 7.5% of outliers
- 7.5% < outliers < 15%
- > 15% of outliers

**Points:descriptors**

- > 10:1 p:d ratio
- 10:1 > p:d ratio > 3:1
- p:d ratio < 3:1

**VERIFY tests**

- Up to ●●●● (tests pass)
- (all tests failed)

### Some tips to improve the score

- ✓ A ROBERT score of 9 or 10 suggests that the predictive ability of your model is strong, congratulations!

### How to predict new values with these models?

1. Create a CSV database with the new points, including the necessary descriptors.
2. Place the CSV file in the parent folder (i.e., where the module folders were created)
3. Run the PREDICT module as 'python -m robert --predict --csv\_test FILENAME.csv'.
4. The predictions will be shown at the end of the resulting PDF report and will be stored in the last column of two CSV files called MODEL\_SIZE\_test(\_No)\_PFI.csv, which are in the PREDICT folder.



## REPRODUCIBILITY

*This section provides all the instructions to reproduce the results presented.*

### **1. Download these files (*the authors should have uploaded the files as supporting information!*):**

- CSV database (bmc\_dft\_robert\_input\_NBOonly\_top08.csv)

### **2. Install and adjust the versions of the following Python modules:**

- Install ROBERT and its dependencies: `conda install -c conda-forge robert`
- Adjust ROBERT version: `pip install robert==1.0.6`
- Install scikit-learn-intelex: `pip install scikit-learn-intelex==2024.4.0`

*(if scikit-learn-intelex is not installed, slightly different results might be obtained)*

### **3. Run ROBERT using this command line in the folder with the CSV database:**

```
python -m robert --y "dG_C5" --names "Cofactor" --csv_name "bmc_dft_robert_input_NBOonly_top08.csv" --ignore "[Cofactor]" --model "[MVL]" --train "[85]"
```

### **4. Execution time, Python version and OS:**

Originally run in Python 3.10.14 using Linux #1 SMP Tue Oct 19 15:14:17 UTC 2021

Total execution time: 7.45 seconds (*the number of processors should be specified by the user*)



## TRANSPARENCY

*This section contains important parameters used in scikit-learn models and ROBERT.*

### 1. Parameters of the scikit-learn models (same keywords as used in scikit-learn):

#### No PFI (all descriptors):

sklearn model: LinearRegression  
random\_state: 8  
names: Cofactor

#### PFI (only important descriptors):

sklearn model: LinearRegression  
random\_state: 43  
names: Cofactor

### 2. ROBERT options for data split (KN or RND), predict type (REG or CLAS) and hyperopt error (RMSE, etc.):

#### No PFI (all descriptors):

split: RND  
type: reg  
error\_type: rmse

#### PFI (only important descriptors):

split: RND  
type: reg  
error\_type: rmse



## ABBREVIATIONS

*Reference section for the abbreviations used.*

**ACC:** accuracy

**ADAB:** AdaBoost

**CSV:** comma separated values

**CLAS:** classification

**CV:** cross-validation

**F1 score:** balanced F-score

**GB:** gradient boosting

**GP:** gaussian process

**KN:** k-nearest neighbors

**MAE:** root-mean-square error

**MCC:** Matthew's correl. coefficient

**ML:** machine learning

**MVL:** multivariate lineal models

**NN:** neural network

**PFI:** permutation feature importance

**R2:** coefficient of determination

**REG:** Regression

**RF:** random forest

**RMSE:** root mean square error

**RND:** random

**SHAP:** Shapley additive explanations

**VR:** voting regressor

**CURATE**

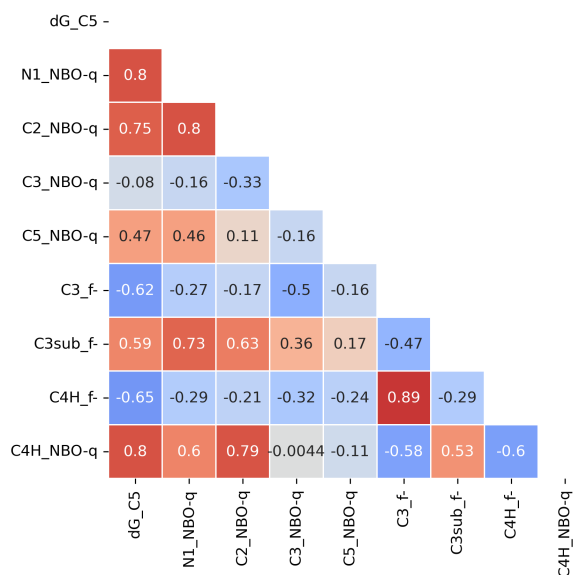
*This module takes care of data curation, including filters for correlated descriptors, noise, and duplicates, as well as conversion of categorical descriptors.*

The complete output (CURATE\_data.dat) and curated database are stored in the CURATE folder.

Time CURATE: 0.35 seconds

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

**Pearson's r heatmap**

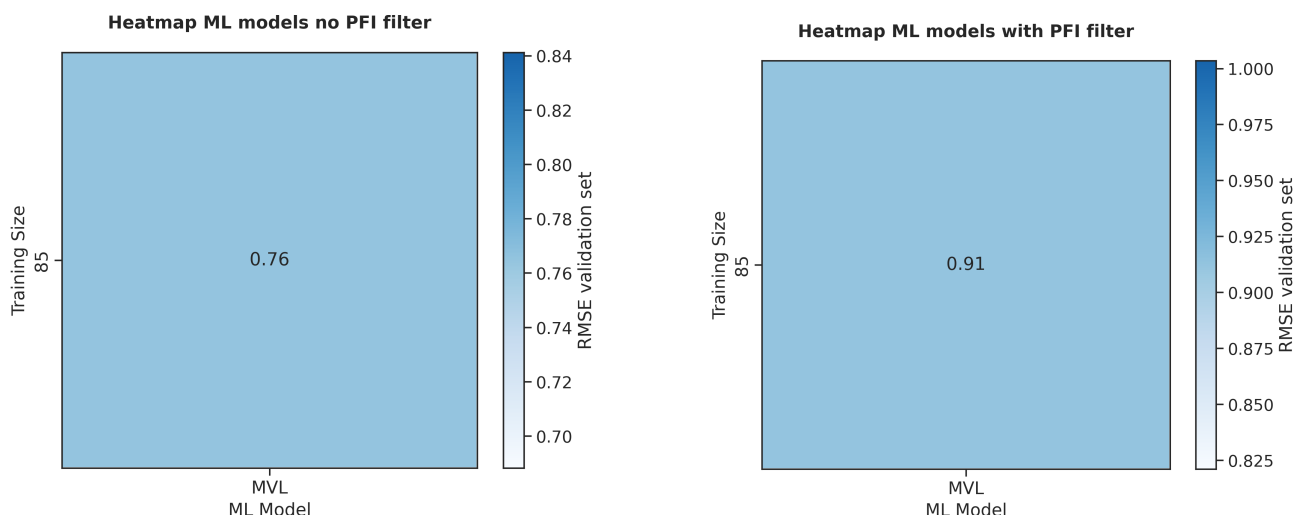
**GENERATE**

*This module carries out a screening of ML models and selects the most accurate one. It includes a comparison of multiple hyperoptimized models and training sizes.*

The complete output (GENERATE\_data.dat) and heatmaps are stored in the GENERATE folder.

Time GENERATE: 0.99 seconds

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



## VERIFY

Determination of predictive ability of models using four tests: 5-fold CV, y-mean (error against the mean y baseline), y-shuffle (predict with shuffled y values), and one-hot (predict using one-hot encoding instead of the X values).

The complete output (VERIFY\_data.dat) and donut plot are stored in the VERIFY folder.

Time VERIFY: 0.69 seconds

### ----- Images and summary generated by the VERIFY module -----

#### No PFI (all descriptors):

Original RMSE (valid. set)  $0.76 + 25\% \text{ thres.} = 0.96$

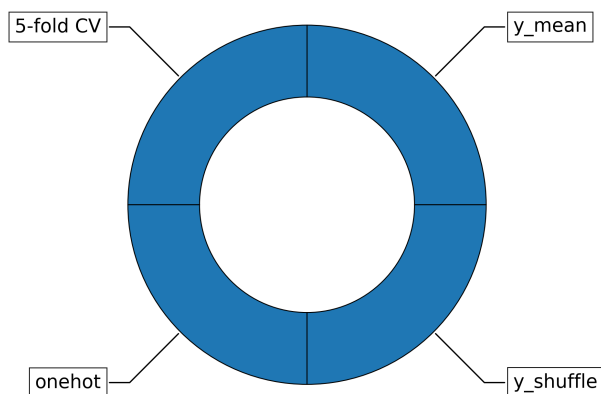
- o 5-fold CV: PASSED, RMSE = 0.89, lower than thres.
- o y\_mean: PASSED, RMSE = 3.7, higher than thres.
- o y\_shuffle: PASSED, RMSE = 6.0, higher than thres.
- o onehot: PASSED, RMSE = 3.7, higher than thres.

#### PFI (only important descriptors):

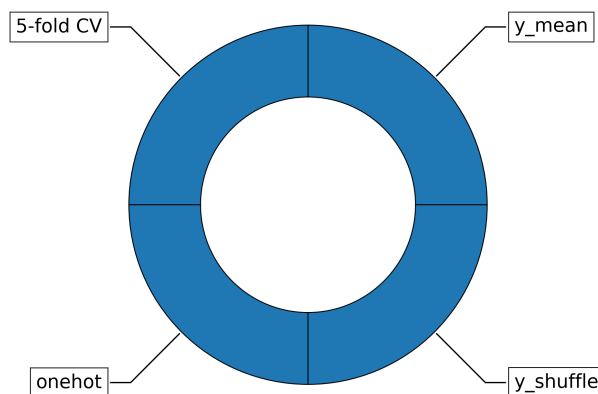
Original RMSE (valid. set)  $0.91 + 25\% \text{ thres.} = 1.1$

- o 5-fold CV: PASSED, RMSE = 0.94, lower than thres.
- o y\_mean: PASSED, RMSE = 4.8, higher than thres.
- o y\_shuffle: PASSED, RMSE = 6.8, higher than thres.
- o onehot: PASSED, RMSE = 4.9, higher than thres.

**VERIFY tests of MVL\_85\_No\_PFI**



**VERIFY tests of MVL\_85\_PFI**





## PREDICT

This module predicts and plots the results of training and validation sets from GENERATE, as well as from external test sets (if any). Feature importances from SHAP and PFI, and outlier analysis are also represented.

The complete output (PREDICT\_data.dat) and heatmaps are stored in the PREDICT folder.

Time PREDICT: 5.42 seconds

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

#### No PFI (all descriptors):

##### Prediction metrics and descriptors

- Points Train:Validation:Test = 101:18:13
- Proportion Train:Validation:Test = 77:14:10
- Number of descriptors = 8
- Proportion (train+valid.) points:descriptors = 119:8
- Train :  $R^2 = 0.97$ , MAE = 0.64, RMSE = 0.89
- Valid. :  $R^2 = 0.96$ , MAE = 0.59, RMSE = 0.76
- Test :  $R^2 = 0.98$ , MAE = 0.61, RMSE = 0.7

##### Outliers (max. 10 shown)

Train: 6 outliers out of 101 datapoints (5.9%)

- BMC\_009 (4.0 SDs)
- BMC\_039 (2.5 SDs)
- BMC\_046 (2.4 SDs)
- BMC\_113 (4.3 SDs)
- BMC\_114 (2.4 SDs)
- BMC\_124 (2.2 SDs)

Validation: 0 outliers out of 18 datapoints (0.0%)

Test: 0 outliers out of 13 datapoints (0.0%)

#### PFI (only important descriptors):

##### Prediction metrics and descriptors

- Points Train:Validation:Test = 101:18:13
- Proportion Train:Validation:Test = 77:14:10
- Number of descriptors = 5
- Proportion (train+valid.) points:descriptors = 119:5
- Train :  $R^2 = 0.96$ , MAE = 0.65, RMSE = 0.92
- Valid. :  $R^2 = 0.97$ , MAE = 0.67, RMSE = 0.91
- Test :  $R^2 = 0.98$ , MAE = 0.52, RMSE = 0.64

##### Outliers (max. 10 shown)

Train: 6 outliers out of 101 datapoints (5.9%)

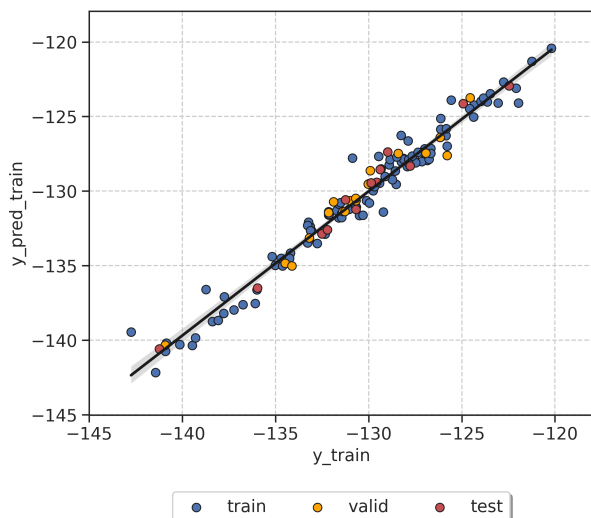
- BMC\_009 (4.5 SDs)
- BMC\_010 (2.0 SDs)
- BMC\_032 (2.1 SDs)
- BMC\_039 (2.4 SDs)
- BMC\_042 (2.0 SDs)
- BMC\_113 (4.2 SDs)

Validation: 1 outliers out of 18 datapoints (5.6%)

- BMC\_124 (2.5 SDs)

Test: 0 outliers out of 13 datapoints (0.0%)

Predictions\_train\_valid\_test of MVL\_85\_No\_PFI



Predictions\_train\_valid\_test of MVL\_85\_PFI

