ROBERT v 1.0.6 2025/02/04 09:27:44

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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: NN
Proportion Train:Validation = 90:10

WEAK

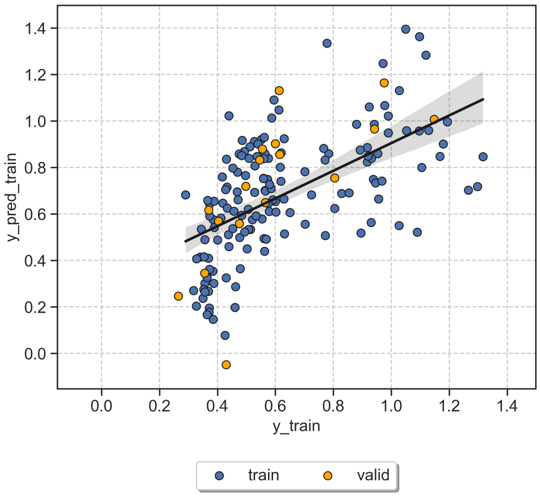
The model has a score of 5/10

- The valid. set shows an R^2 of 0.5

● The valid. set has 11.8% of outliers

●● Using 166:8 points(train+valid.):descriptors

●● The valid. set passes 2 VERIFY tests



Train : R^2 = 0.35, MAE = 0.19, RMSE = 0.24
Valid. : R^2 = 0.5, MAE = 0.2, RMSE = 0.25

PFI (only important descriptors):

ML model: NN
Proportion Train:Validation = 90:10

MODERATE

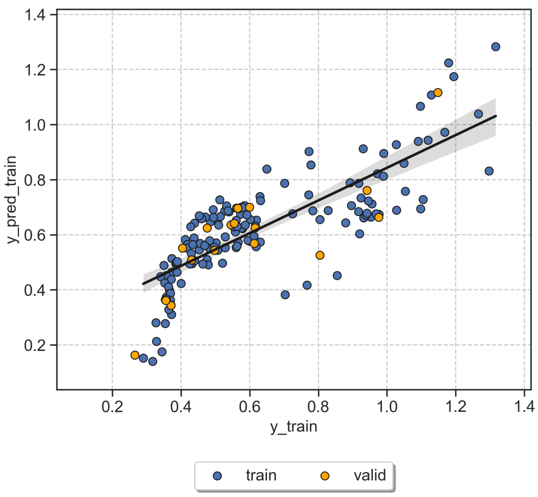
The model has a score of 8/10

- The valid. set shows an R^2 of 0.66

●● The valid. set has 5.9% of outliers

●● Using 166:4 points(train+valid.):descriptors

●●●● The valid. set passes 4 VERIFY tests



Train : R^2 = 0.64, MAE = 0.12, RMSE = 0.15
Valid. : R^2 = 0.66, MAE = 0.11, RMSE = 0.14

Score thresholds *(detailed in https://robert.readthedocs.io/en/latest/Score/score.html)*

R^2	Outliers	Points:descriptors	VERIFY tests
●● $R^2 > 0.85$	●● < 7.5% of outliers	●● > 10:1 p:d ratio	Up to ●●●● (tests pass)
● $0.85 > R^2 > 0.70$	● 7.5% < outliers < 15%	● 10:1 > p:d ratio > 3:1	- (all tests failed)
- $R^2 < 0.70$	- > 15% of outliers	- p:d ratio < 3:1	

Some tips to improve the score

⚠ One of your models have more than 7.5% of outliers (5% is expected for a normal distribution with the t-value of 2 that ROBERT uses), using a more homogeneous distribution of results might help.

⚠ Replacing or deleting the least useful descriptors used might help to improve the model. Feature importances are gathered in the SHAP and PFI sections of the /PREDICT/PREDICT_data.dat file.

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 (smooth_sin_rGO_sin_DMF_clima_noise_ratio_m16.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
- scikit-learn-intelex: not installed

(if scikit-learn-intelex is installed, slightly different results might be obtained)

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

```
python -m robert --model "[NN]" --train "[90]" --ignore "[indice,area,cell]" --names "indice" --y "PCE" --auto_test
"False" --csv_name "smooth_sin_rGO_sin_DMF_clima_noise_ratio_m16.csv"
```

4. Execution time, Python version and OS:

Originally run in Python 3.10.12 using Darwin Darwin Kernel Version 22.5.0: Thu Jun 8 22:22:19 PDT 2023; root:xnu-8796.121.3~7/R

Total execution time: 23.46 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):	**PFI (only important descriptors):**
sklearn model: MLPRegressor	sklearn model: MLPRegressor
random_state: 70	random_state: 70
names: indice	names: indice
batch_size: 4	batch_size: 4
hidden_layer_sizes: [32]	hidden_layer_sizes: [32]
learning_rate_init: 0.01	learning_rate_init: 0.01
max_iter: 200	max_iter: 200
validation_fraction: 0.3	validation_fraction: 0.3
alpha: 0.0001	alpha: 0.0001
shuffle: False	shuffle: False
tol: 0.0001	tol: 0.0001
early_stopping: False	early_stopping: False
beta_1: 0.999	beta_1: 0.999
beta_2: 0.999	beta_2: 0.999
epsilon: 1e-08	epsilon: 1e-08

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

No PFI (all descriptors):	**PFI (only important descriptors):**
split: RND	split: RND
type: reg	type: reg
error_type: rmse	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

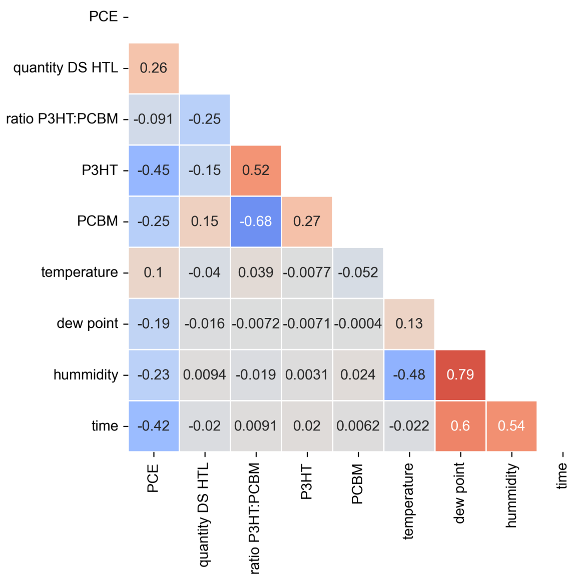
This module takes care of data curation, including filters for correlated descriptors, noise, and duplicates, as well as conversion of categorical descriptors.

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

Time CURATE: 0.3 seconds

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

Pearson's r heatmap



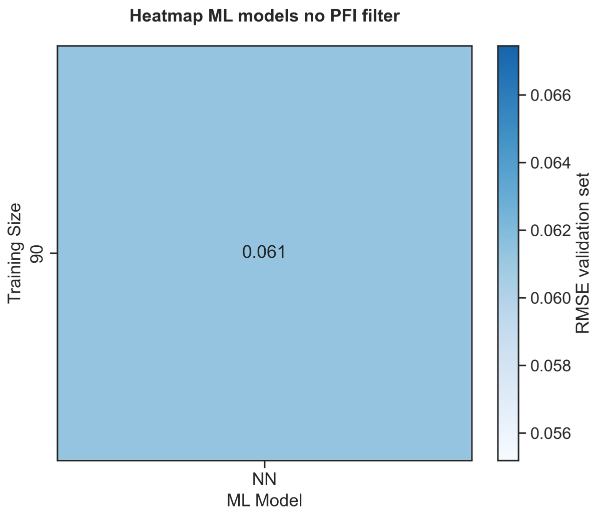
GENERATE

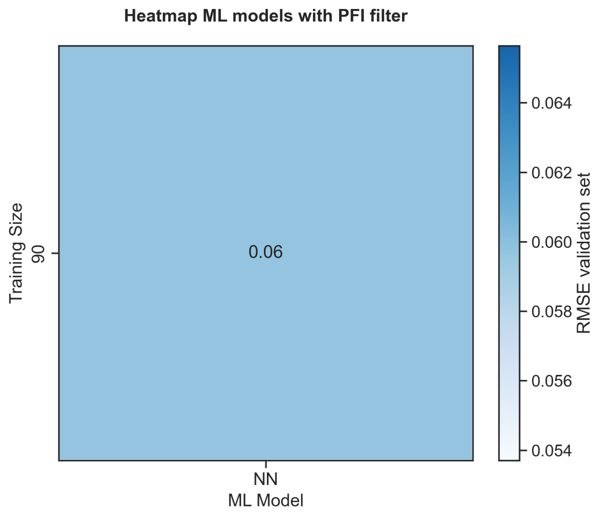
This module carries out a screening of ML models and selects the most accurate one. It includes a comparison of multiple hyperoptimized models and training sizes.

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

Time GENERATE: 17.76 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: 2.3 seconds

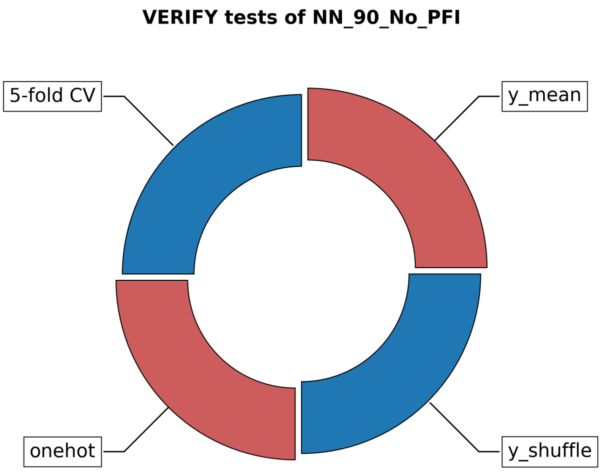
------- Images and summary generated by the VERIFY module -------

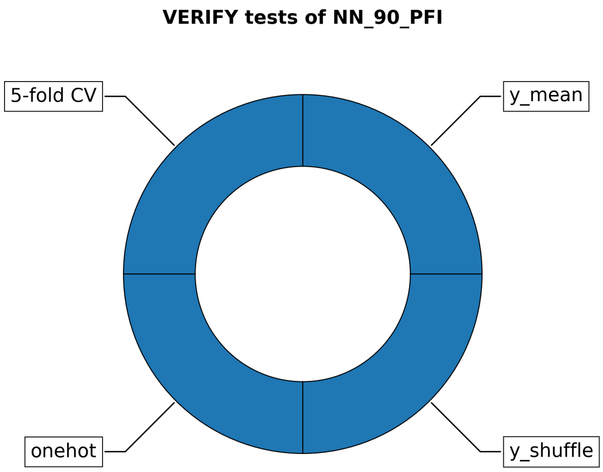
No PFI (all descriptors):

Original RMSE (valid. set) 0.25 + 25% thres. = 0.31
o 5-fold CV: PASSED, RMSE = 0.17, lower than thres.
x y_mean: FAILED, RMSE = 0.23, lower than thres.
o y_shuffle: PASSED, RMSE = 0.4, higher than thres.
x onehot: FAILED, RMSE = 0.26, lower than thres.

PFI (only important descriptors):

Original RMSE (valid. set) 0.14 + 25% thres. = 0.17
o 5-fold CV: PASSED, RMSE = 0.11, lower than thres.
o y_mean: PASSED, RMSE = 0.23, higher than thres.
o y_shuffle: PASSED, RMSE = 0.3, higher than thres.
o onehot: PASSED, RMSE = 0.24, higher than thres.





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: 3.1 seconds

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

No PFI (all descriptors):

Prediction metrics and descriptors

- Points Train:Validation = 149:17
- Proportion Train:Validation = 90:10
- Number of descriptors = 8
- Proportion (train+valid.) points:descriptors = 166:8
- Train : R^2 = 0.35, MAE = 0.19, RMSE = 0.24
- Valid. : R^2 = 0.5, MAE = 0.2, RMSE = 0.25

Outliers (max. 10 shown)

Train: 7 outliers out of 149 datapoints (4.7%)

- 3 (2.8 SDs)
- 4 (2.7 SDs)
- 5 (2.7 SDs)
- 8 (2.0 SDs)
- 16 (2.6 SDs)
- 38 (2.2 SDs)
- 61 (2.8 SDs)

Validation: 2 outliers out of 17 datapoints (11.8%)

- 30 (2.3 SDs)
- 156 (2.1 SDs)

PFI (only important descriptors):

Prediction metrics and descriptors

- Points Train:Validation = 149:17
- Proportion Train:Validation = 90:10
- Number of descriptors = 4
- Proportion (train+valid.) points:descriptors = 166:4
- Train : R^2 = 0.64, MAE = 0.12, RMSE = 0.15
- Valid. : R^2 = 0.66, MAE = 0.11, RMSE = 0.14

Outliers (max. 10 shown)

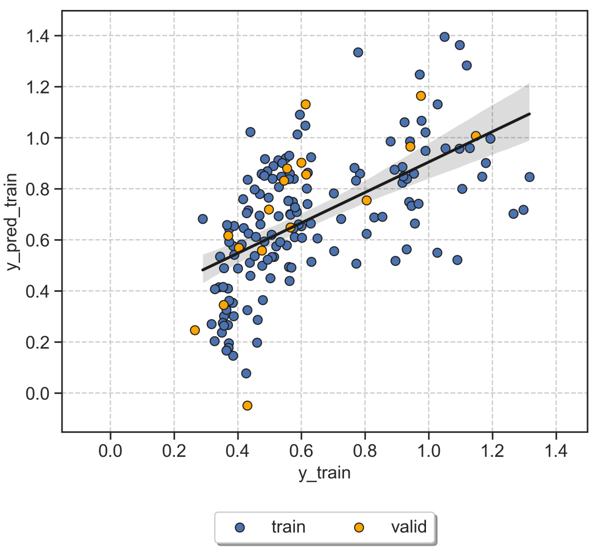
Train: 8 outliers out of 149 datapoints (5.4%)

- 3 (3.7 SDs)
- 10 (2.7 SDs)
- 11 (3.0 SDs)
- 15 (2.3 SDs)
- 142 (2.1 SDs)
- 154 (3.0 SDs)
- 159 (2.4 SDs)
- 163 (2.1 SDs)

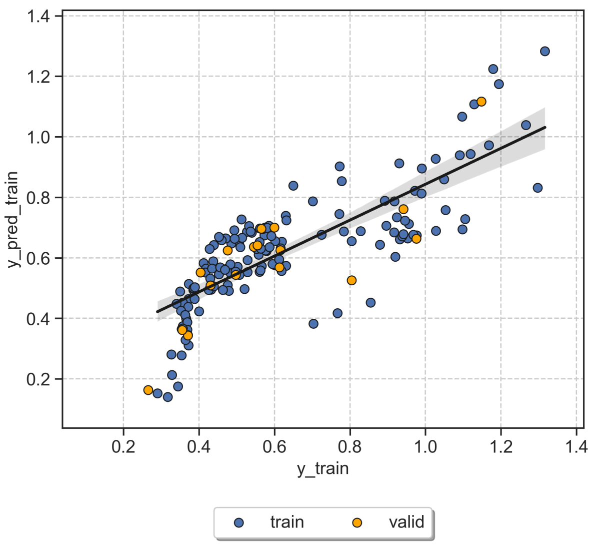
Validation: 1 outliers out of 17 datapoints (5.9%)

- 29 (2.0 SDs)

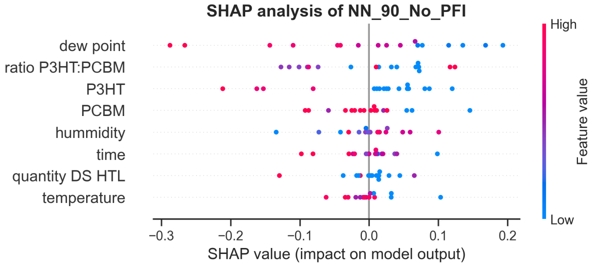
Predictions_train_valid of NN_90_No_PFI



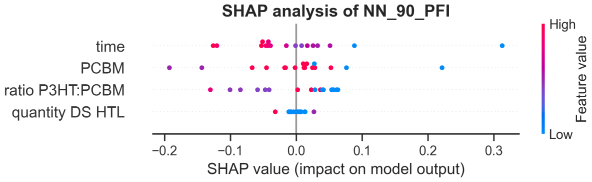
Predictions_train_valid of NN_90_PFI



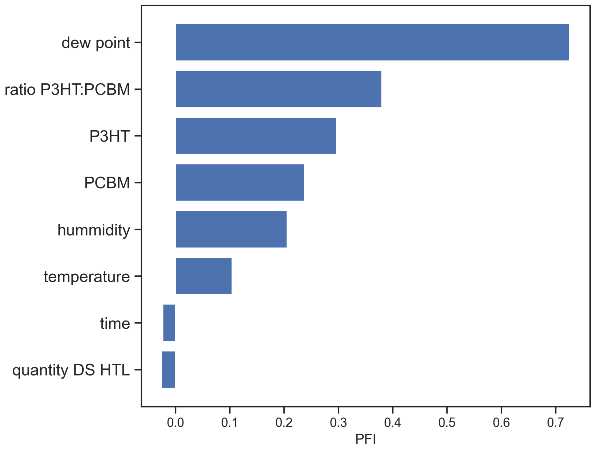
SHAP analysis of NN_90_No_PFI



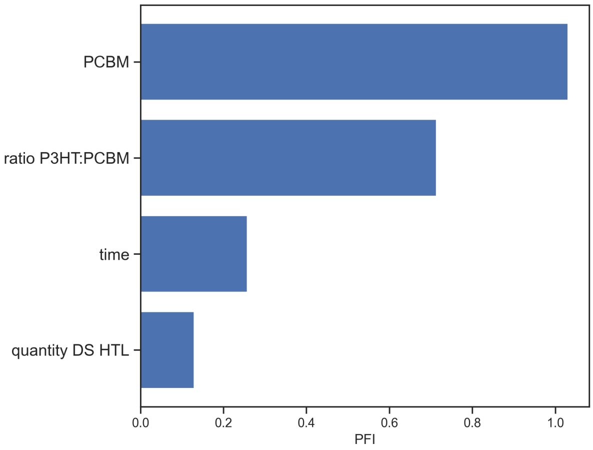
SHAP analysis of NN_90_PFI



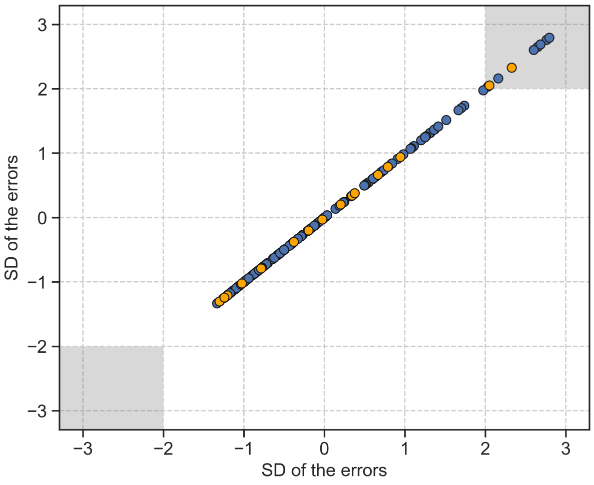
Permutation feature importances (PFIs) of NN_90_No_PFI



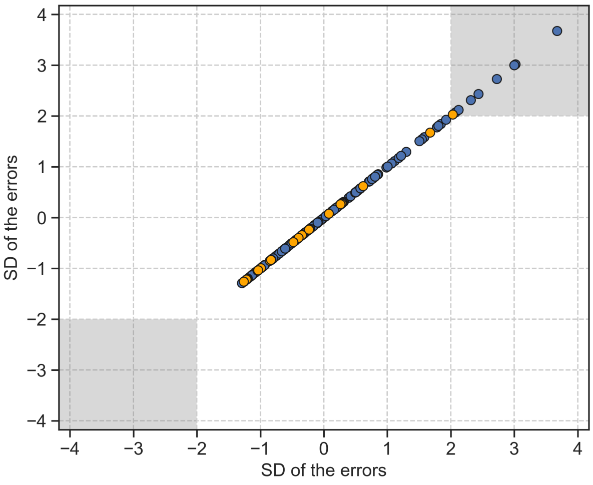
Permutation feature importances (PFIs) of NN_90_PFI



Outlier analysis of NN_90_No_PFI



Outlier analysis of NN_90_PFI


SD of the errors
SD of the errors