Report

ROBERT v 0.0.1 2023/05/02 20:47:18
Citation: ROBERT v 0.0.1, Dalmau, D.; Alegre-Requena, J. V., 2023. https://github.com/jvalegre/robert

Command line used in ROBERT: robert --ignore ['solvent','sample'] --y dG --csv_name Bandar_db.csv --epoch 10 --pfi_max 2 --train [60,70,80]

CURATE

o Starting data curation with the CURATE module

o Database Bandar_db.csv loaded successfully, including:

- 20 datapoints
- 18 accepted descriptors
- 2 ignored descriptors
- 0 discarded descriptors

o Analyzing categorical variables

- No categorical variables were found.

o Duplication filters activated
Excluded datapoints:

o Correlation filter activated with these thresholds: thres_x = 0.85, thres_y = 0.02
Excluded descriptors:

- n: R**2 = 0.02 with the dG values
- Sig3: R**2 = 0.89 with beta
- Hbond_acc: R**2 = 0.91 with beta
- B: R**2 = 0.99 with beta
- MV_boltz: R**2 = 0.0 with the dG values
- area: R**2 = 0.02 with the dG values
- volume: R**2 = 0.01 with the dG values
- V: R**2 = 0.01 with the dG values

o 12 columns remaining after applying correlation filters:

- solvent
- dG
- beta
- gamma
- dielectric
- dispersion
- polar
- hydrogen
- sum
- dipole
- Sig2
- sample

o The Pearson heatmap was stored in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Regression\Bandar\CURATE\Pearson_heatmap.png.

o The curated database was stored in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Regression\Bandar\CURATE\Bandar_db_CURATE.csv.

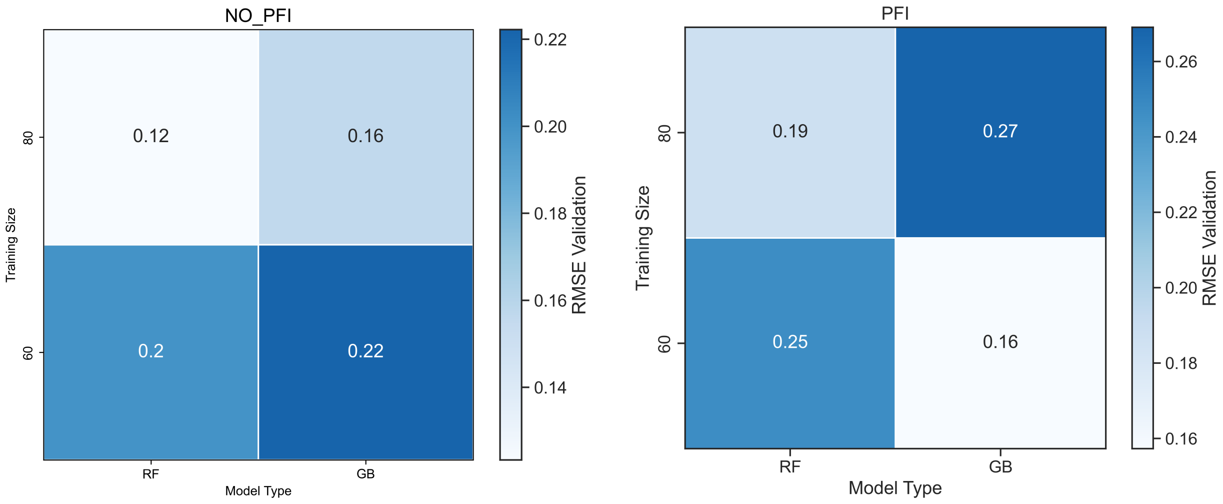
Time CURATE: 0.78 seconds

GENERATE

o Starting generation of ML models with the GENERATE module

o Database C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Regression\Bandar\CURATE\Bandar_db_CURATE.csv loaded successfully, including:
- 20 datapoints
- 10 accepted descriptors
- 2 ignored descriptors
- 0 discarded descriptors

o Starting heatmap scan with 4 ML models ['RF', 'GB', 'NN', 'VR'] and 3 training sizes [60, 70, 80].
Heatmap generation:



PREDICT

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

o ML model NN_60.csv (with no PFI filter) and its corresponding Xy database were loaded successfully, including:
- Target value: dG
- Model: NN
- Descriptors: ['beta', 'gamma', 'dielectric', 'dispersion', 'polar', 'hydrogen', 'sum', 'dipole', 'Sig2']
- Training points: 12
- Validation points: 8
  - Train set with predicted results: NN_60_train_No_PFI.csv

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      -  Validation set with predicted results: NN_60_valid_No_PFI.csv

   o  Saving graphs and CSV databases in C:\Users\David\Desktop\Art�culo ROBERT\
Pruebas_ROBERT\Regression\Bandar\PREDICT:
      -  Graph in: C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Regress
ion\Bandar\PREDICT/Results_NN_60_No_PFI.png

   o  Results saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Reg
ression\Bandar\PREDICT/Results_NN_60_No_PFI.dat:
      -  Points Train:Validation = 12:8
      -  Proportion Train:Validation = 60:40
      -  Train : R2 = 0.51, MAE = 0.32, RMSE = 0.4
      -  Validation : R2 = 0.51, MAE = 0.18, RMSE = 0.23

   o  SHAP plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\R
egression\Bandar\PREDICT/SHAP_NN_60_No_PFI.png
   o  SHAP values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT
\Regression\Bandar\PREDICT/SHAP_NN_60_No_PFI.dat:
      -  gamma = min: -0.24, max: 0.21
      -  beta = min: -0.12, max: 0.19
      -  Sig2 = min: -0.043, max: 0.13
      -  dispersion = min: -0.052, max: 0.13
      -  polar = min: -0.088, max: 0.081
      -  dipole = min: -0.029, max: 0.063
      -  dielectric = min: -0.071, max: 0.059
      -  sum = min: -0.045, max: 0.042
      -  hydrogen = min: -0.014, max: 0.0088

   o  PFI plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Re
gression\Bandar\PREDICT/PFI_NN_60_No_PFI.png
   o  PFI values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\
Regression\Bandar\PREDICT/PFI_NN_60_No_PFI.dat:
      Original score (from model.score, R2) = 0.5
      -  gamma = 1.2 +- 0.6
      -  beta = 0.19 +- 0.22
      -  dielectric = 0.14 +- 0.24
      -  dipole = 0.13 +- 0.13
      -  Sig2 = 0.098 +- 0.051
      -  sum = 0.065 +- 0.081
      -  polar = 0.011 +- 0.18
      -  hydrogen = 0.0082 +- 0.022
      -  dispersion = -0.11 +- 0.09

   o  Outliers plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBE
RT\Regression\Bandar\PREDICT/Outliers_NN_60_No_PFI.png
   o  Outlier values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROB
ERT\Regression\Bandar\PREDICT/Outliers_NN_60_No_PFI.dat:
      x  No variable names found or names option not specified! Outliers will be
 printed with no names
      Train: 1 outliers out of 12 datapoints (8.3%)
      Validation: 0 outliers out of 8 datapoints (0.0%)

o  ML model NN_60_PFI.csv (with PFI filter) and its corresponding Xy database we
re loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma']
   - Training points: 12
   - Validation points: 8
      -  Train set with predicted results: NN_60_train_PFI.csv
      -  Validation set with predicted results: NN_60_valid_PFI.csv

   o  Saving graphs and CSV databases in C:\Users\David\Desktop\Art�culo ROBERT\
Pruebas_ROBERT\Regression\Bandar\PREDICT:
      -  Graph in: C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Regress
ion\Bandar\PREDICT/Results_NN_60_PFI.png

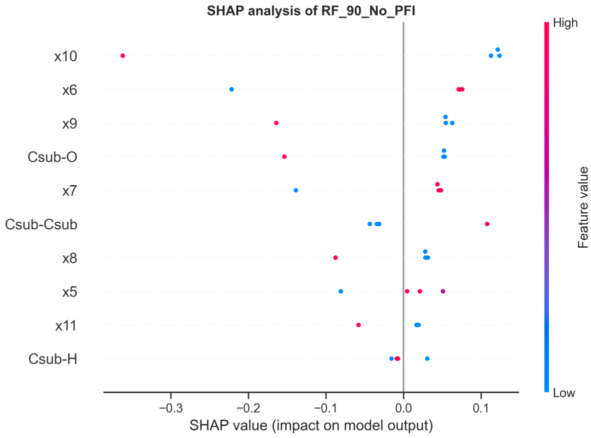
   o  Results saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Reg
ression\Bandar\PREDICT/Results_NN_60_PFI.dat:
      -  Points Train:Validation = 12:8
      -  Proportion Train:Validation = 60:40
      -  Train : R2 = 0.47, MAE = 0.28, RMSE = 0.39
      -  Validation : R2 = 0.6, MAE = 0.18, RMSE = 0.21

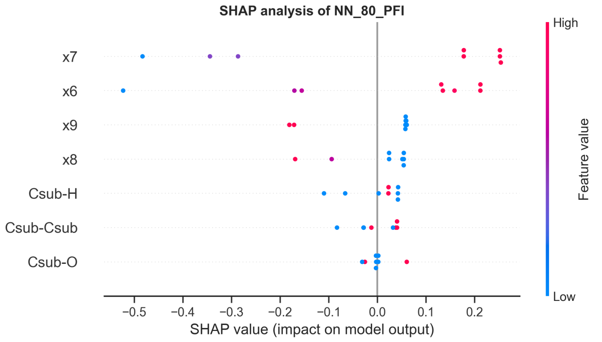
   o  SHAP plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\R
egression\Bandar\PREDICT/SHAP_NN_60_PFI.png
   o  SHAP values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT
\Regression\Bandar\PREDICT/SHAP_NN_60_PFI.dat:
      -  beta = min: -0.21, max: 0.4
      -  gamma = min: -0.22, max: 0.24

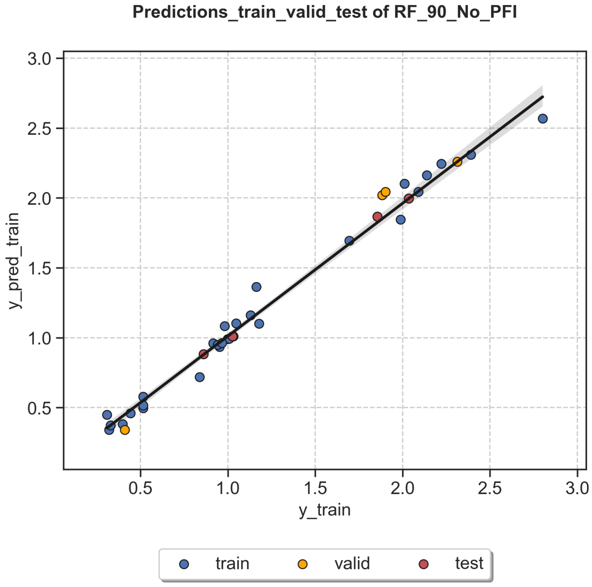
   o  PFI plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\Re
gression\Bandar\PREDICT/PFI_NN_60_PFI.png
   o  PFI values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBERT\
Regression\Bandar\PREDICT/PFI_NN_60_PFI.dat:
      Original score (from model.score, R2) = 0.58
      -  beta = 0.55 +- 0.25
      -  gamma = 0.51 +- 0.3

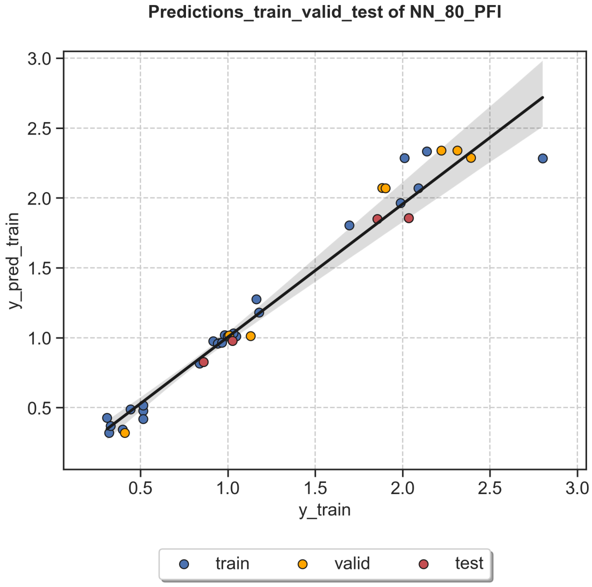
   o  Outliers plot saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROBE
RT\Regression\Bandar\PREDICT/Outliers_NN_60_PFI.png
   o  Outlier values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas_ROB
ERT\Regression\Bandar\PREDICT/Outliers_NN_60_PFI.dat:
      x  No variable names found or names option not specified! Outliers will be
 printed with no names
      Train: 1 outliers out of 12 datapoints (8.3%)
      Validation: 0 outliers out of 8 datapoints (0.0%)

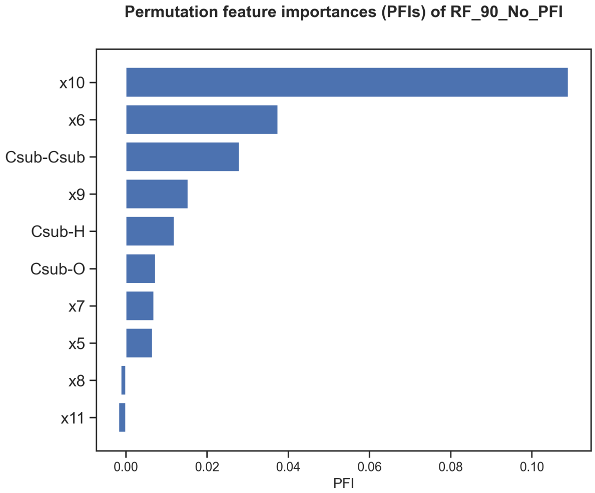
Time PREDICT: 8.72 seconds
```

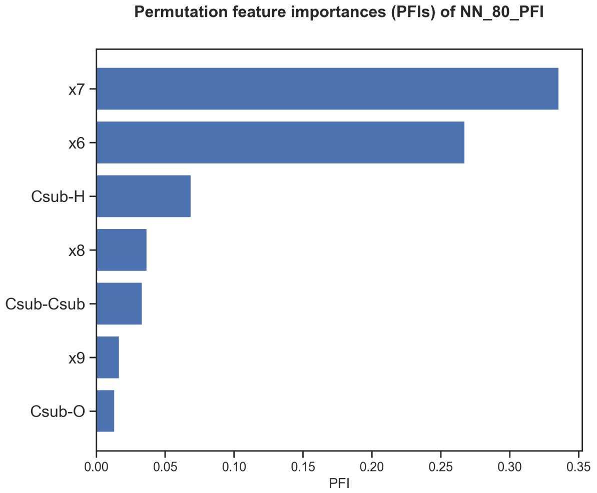












VERIFY

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

o ML model NN_60.csv (with no PFI filter) and its corresponding Xy database were loaded successfully, including:

```
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma', 'dielectric', 'dispersion', 'polar', 'hydrog
en', 'sum', 'dipole', 'Sig2']
   - Training points: 12
   - Validation points: 8

o  ML model NN_60.csv (with no PFI filter) and its corresponding Xy database wer
e loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma', 'dielectric', 'dispersion', 'polar', 'hydrog
en', 'sum', 'dipole', 'Sig2']
   - Training points: 12
   - Validation points: 8

o  ML model NN_60.csv (with no PFI filter) and its corresponding Xy database wer
e loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma', 'dielectric', 'dispersion', 'polar', 'hydrog
en', 'sum', 'dipole', 'Sig2']
   - Training points: 12
   - Validation points: 8

o  ML model NN_60.csv (with no PFI filter) and its corresponding Xy database wer
e loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma', 'dielectric', 'dispersion', 'polar', 'hydrog
en', 'sum', 'dipole', 'Sig2']
   - Training points: 12
   - Validation points: 8

   o  VERIFY donut plots saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas
_ROBERT\Regression\Bandar\VERIFY/VERIFY_tests_NN_60_No_PFI.png
   o  VERIFY test values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas
_ROBERT\Regression\Bandar\VERIFY/VERIFY_tests_NN_60_No_PFI.dat:
      Results of the VERIFY tests:
      Original score (train set for CV): RMSE = 0.4, with a +- threshold (thres_
test option) of 20.0%:
         - 5-fold CV: NOT DETERMINED, data splitting was done with KN. CV result
: RMSE = 0.61
      Original score (validation set): RMSE = 0.23, with a +- threshold (thres_t
est option) of 20.0%:
         o X_shuffle: PASSED, RMSE = 0.51 is higher than the threshold (0.27)
         o y_shuffle: PASSED, RMSE = 0.43 is higher than the threshold (0.27)
         o onehot: PASSED, RMSE = 0.46 is higher than the threshold (0.27)

o  ML model NN_60_PFI.csv (with PFI filter) and its corresponding Xy database we
re loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma']
   - Training points: 12
   - Validation points: 8
```

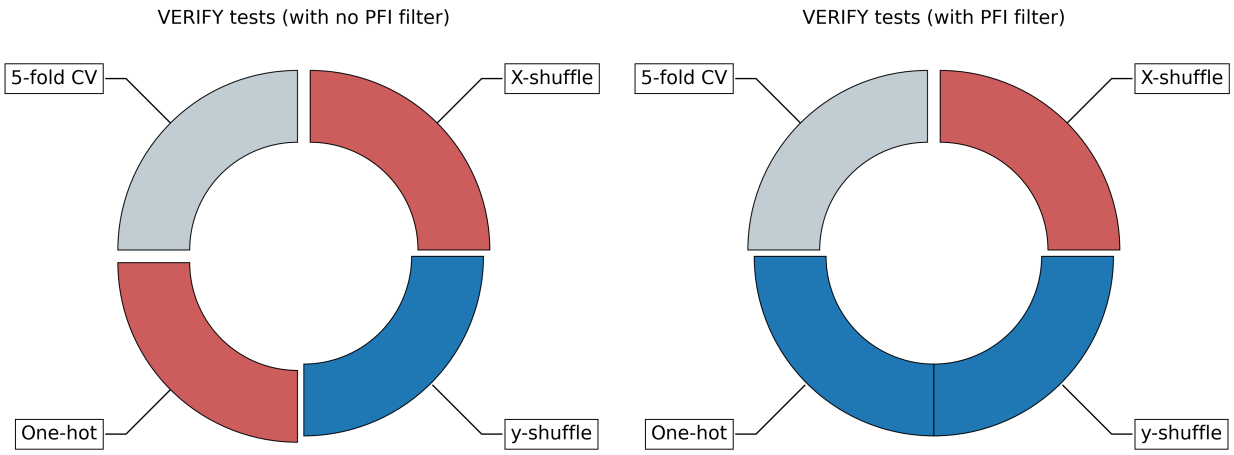
```
o  ML model NN_60_PFI.csv (with PFI filter) and its corresponding Xy database we
re loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma']
   - Training points: 12
   - Validation points: 8

o  ML model NN_60_PFI.csv (with PFI filter) and its corresponding Xy database we
re loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma']
   - Training points: 12
   - Validation points: 8

o  ML model NN_60_PFI.csv (with PFI filter) and its corresponding Xy database we
re loaded successfully, including:
   - Target value: dG
   - Model: NN
   - Descriptors: ['beta', 'gamma']
   - Training points: 12
   - Validation points: 8

   o  VERIFY donut plots saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas
_ROBERT\Regression\Bandar\VERIFY/VERIFY_tests_NN_60_PFI.png
   o  VERIFY test values saved in C:\Users\David\Desktop\Art�culo ROBERT\Pruebas
_ROBERT\Regression\Bandar\VERIFY/VERIFY_tests_NN_60_PFI.dat:
      Results of the VERIFY tests:
      Original score (train set for CV): RMSE = 0.39, with a +- threshold (thres
_test option) of 20.0%:
         - 5-fold CV: NOT DETERMINED, data splitting was done with KN. CV result
: RMSE = 0.5
      Original score (validation set): RMSE = 0.21, with a +- threshold (thres_t
est option) of 20.0%:
         o X_shuffle: PASSED, RMSE = 0.39 is higher than the threshold (0.25)
         o y_shuffle: PASSED, RMSE = 0.31 is higher than the threshold (0.25)
         o onehot: PASSED, RMSE = 0.36 is higher than the threshold (0.25)

Time VERIFY: 1.56 seconds
```



AQME-ROBERT