

# Report



ROBERT v 0.0.1 2023/05/02 20:47:18

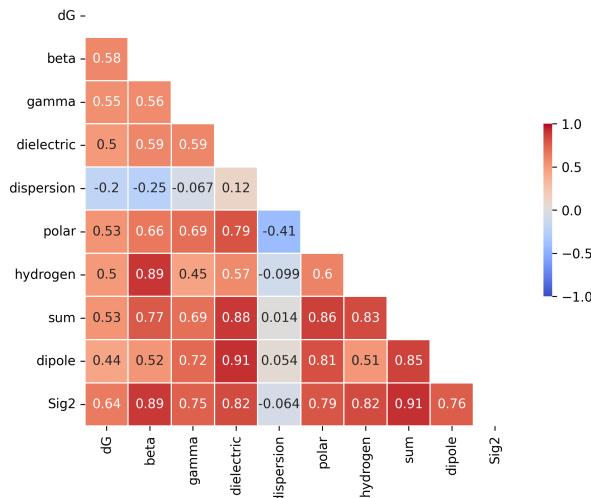
Citation: ROBERT v 0.0.1, Dalmau, D.; Alegre-Requena, J. V., 2023. <https://github.com/jvalegre/robert>

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\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\CURATE\Pearson\_heatmap.png.
- o The curated database was stored in C:\Users\David\Desktop\Artculo 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\Artículo 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]

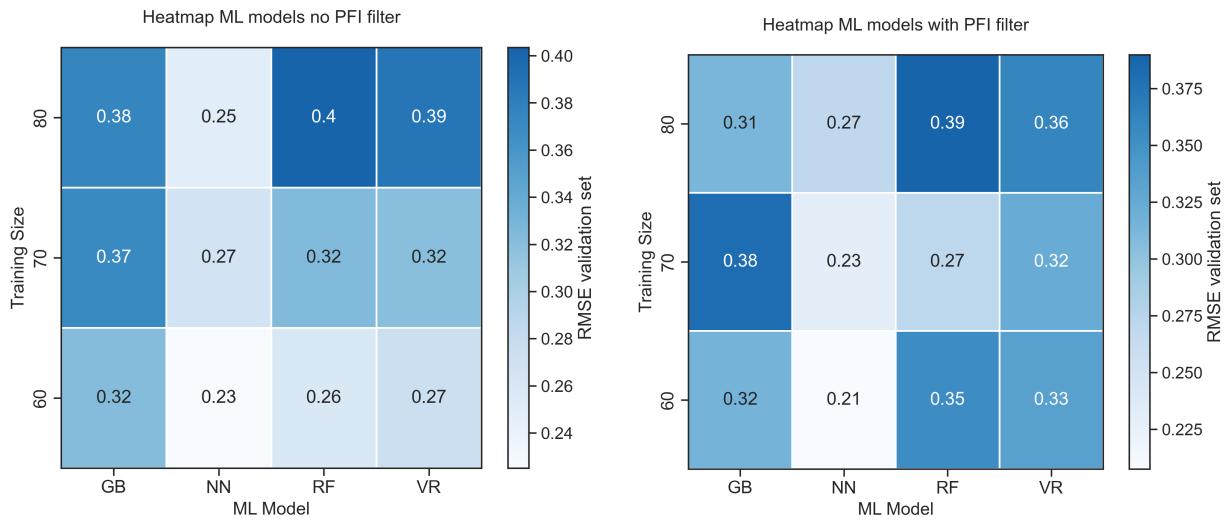
Heatmap generation:

- 1/12
- 2/12
- 3/12
- 4/12
- 5/12
- x The PFI filter was disabled for model GB\_70 (no variables passed)
- 6/12
- 7/12
- 8/12
- x The PFI filter was disabled for model RF\_80 (no variables passed)
- 9/12
- 10/12
- 11/12
- x The PFI filter was disabled for model VR\_80 (no variables passed)
- 12/12

- o Heatmap ML models no PFI filter successfully created in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\GENERATE\Raw\_data

- o Heatmap ML models with PFI filter successfully created in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\GENERATE\Raw\_data

Time GENERATE: 25.03 seconds



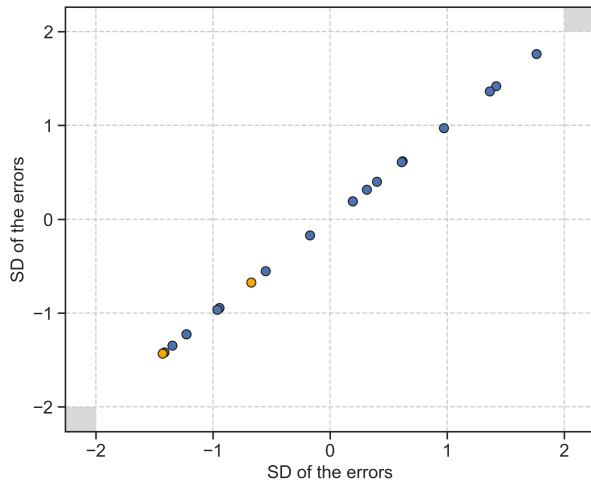
## PREDICT

- 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
    - Validation set with predicted results: NN\_60\_valid\_No\_PFI.csv
- o Saving graphs and CSV databases in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT:
  - Graph in: C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT\Results\_NN\_60\_No\_PFI.png
  - Results saved in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\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\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT\SHAP\_NN\_60\_No\_PFI.png
- o SHAP values saved in C:\Users\David\Desktop\Artículo 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\Artículo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT\PFI\_NN\_60\_No\_PFI.png
- o PFI values saved in C:\Users\David\Desktop\Artículo 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

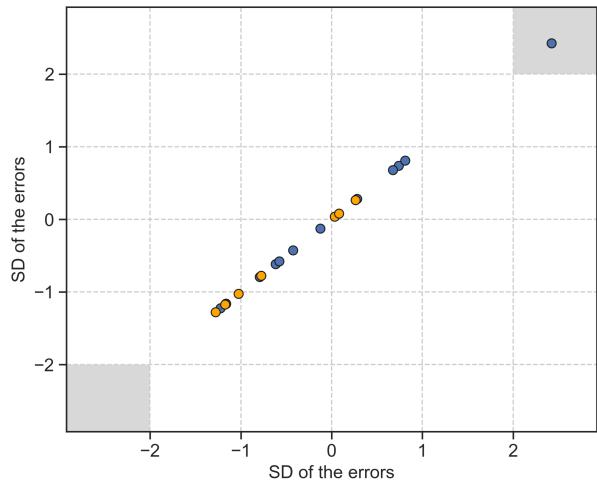
- Sig2 = 0.098 +- 0.051
  - sum = 0.065 +- 0.081
  - polar = 0.011 +- 0.18
  - hydrogen = 0.0082 +- 0.022
  - dispersion = -0.11 +- 0.09
- o Outliers plot saved in C:\Users\David\Desktop\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT\Outliers\_NN\_60\_No\_PFI.png
  - o Outlier values saved in C:\Users\David\Desktop\Artculo ROBERT\Pruebas\_ROBERT\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 were 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\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT:
    - Graph in: C:\Users\David\Desktop\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT/Results\_NN\_60\_PFI.png
- o Results saved in C:\Users\David\Desktop\Artculo ROBERT\Pruebas\_ROBERT\Regression\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\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT/SHAP\_NN\_60\_PFI.png
  - o SHAP values saved in C:\Users\David\Desktop\Artculo 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\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT/PFI\_NN\_60\_PFI.png
  - o PFI values saved in C:\Users\David\Desktop\Artculo 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\Artculo ROBERT\Pruebas\_ROBERT\Regression\Bandar\PREDICT\Outliers\_NN\_60\_PFI.png
  - o Outlier values saved in C:\Users\David\Desktop\Artculo ROBERT\Pruebas\_ROBERT\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

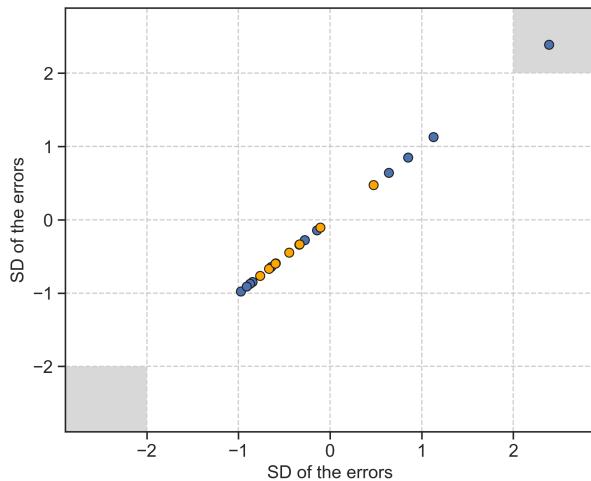
Outlier analysis of GB\_90\_PFI



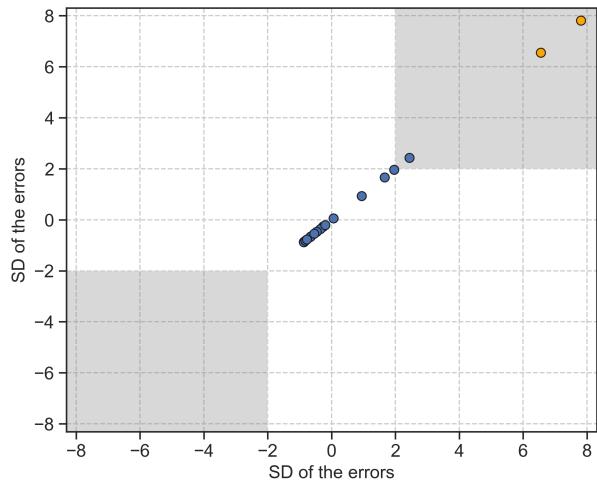
Outlier analysis of NN\_60\_No\_PFI



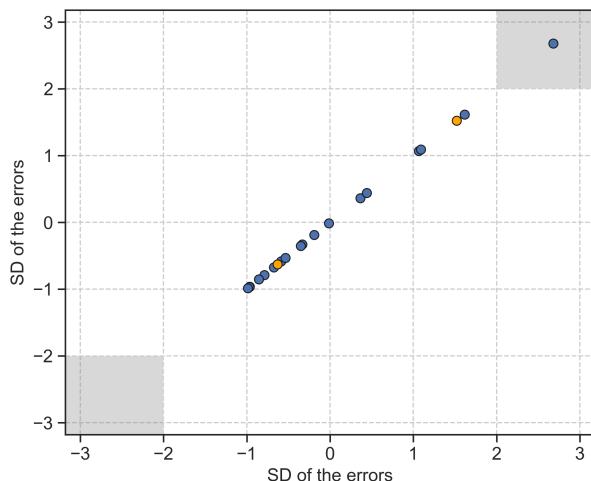
Outlier analysis of NN\_60\_PFI



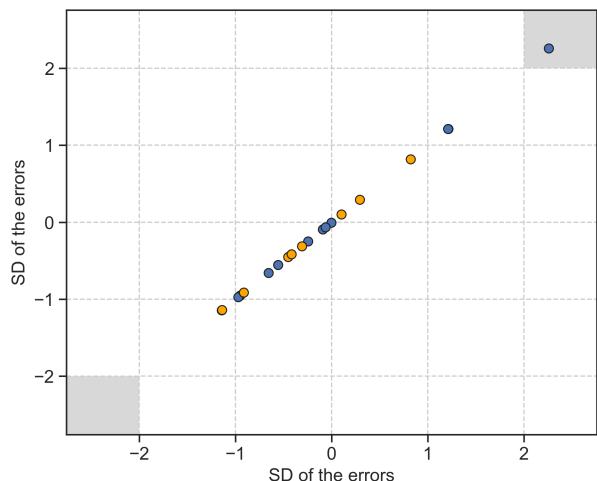
Outlier analysis of NN\_90\_No\_PFI



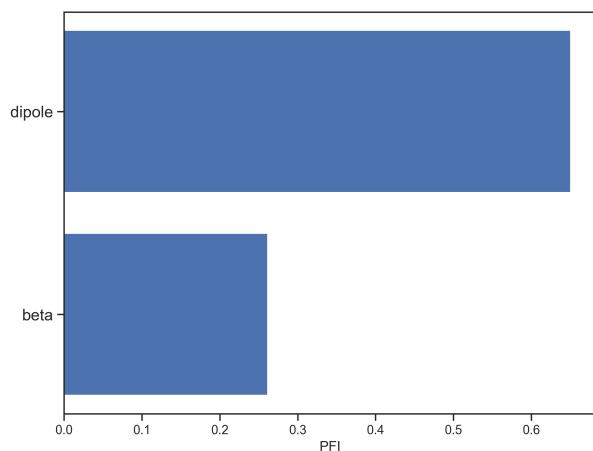
Outlier analysis of NN\_90\_PFI



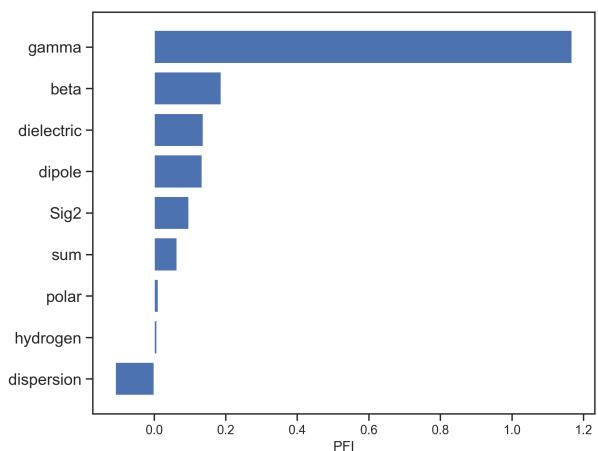
Outlier analysis of VR\_60\_No\_PFI



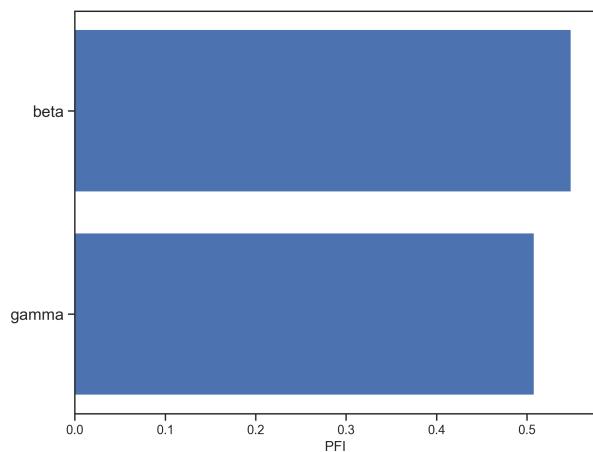
Permutation feature importances (PFI) of GB\_90\_PFI



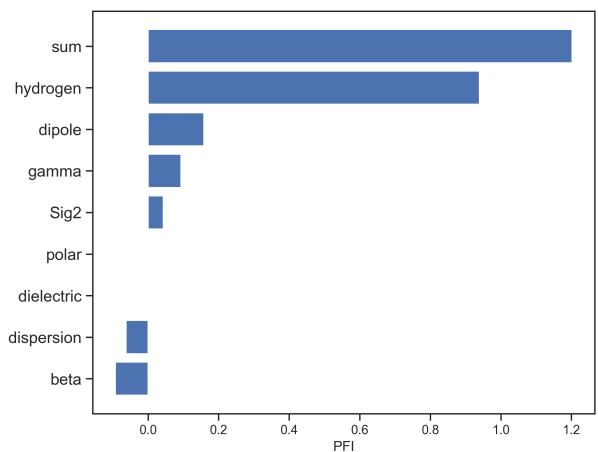
Permutation feature importances (PFI) of NN\_60\_No\_PFI



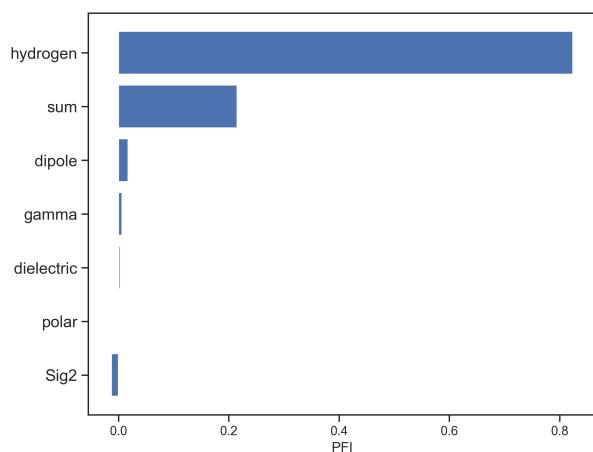
Permutation feature importances (PFI) of NN\_60\_PFI



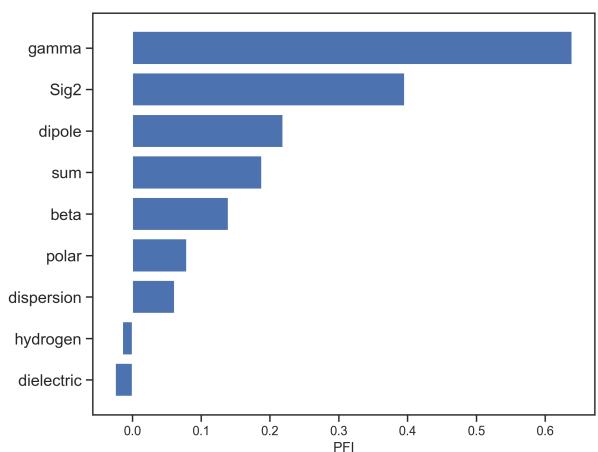
Permutation feature importances (PFI) of NN\_90\_No\_PFI



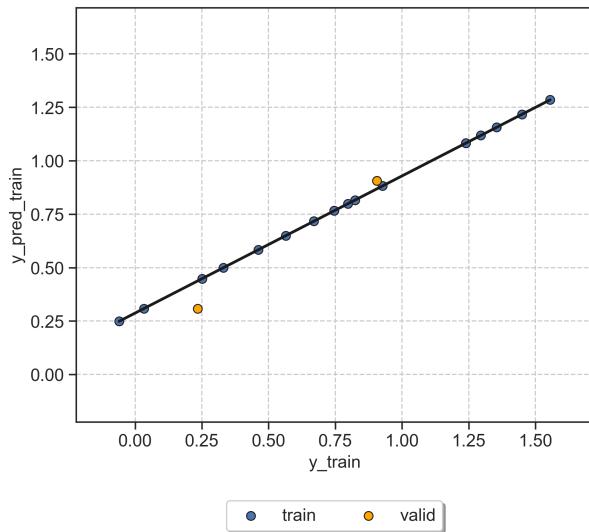
Permutation feature importances (PFI) of NN\_90\_PFI



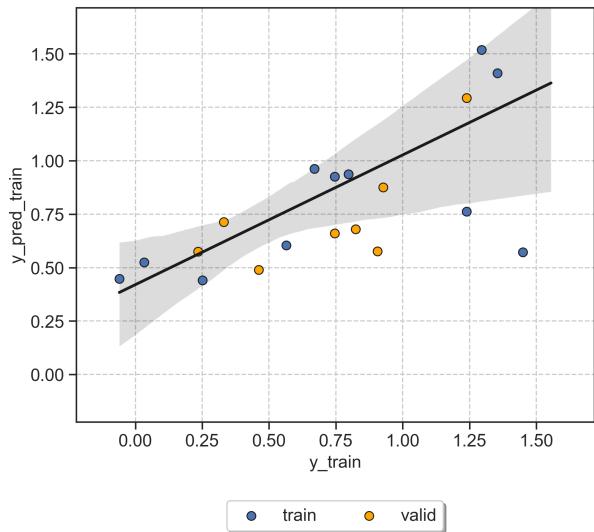
Permutation feature importances (PFI) of VR\_60\_No\_PFI



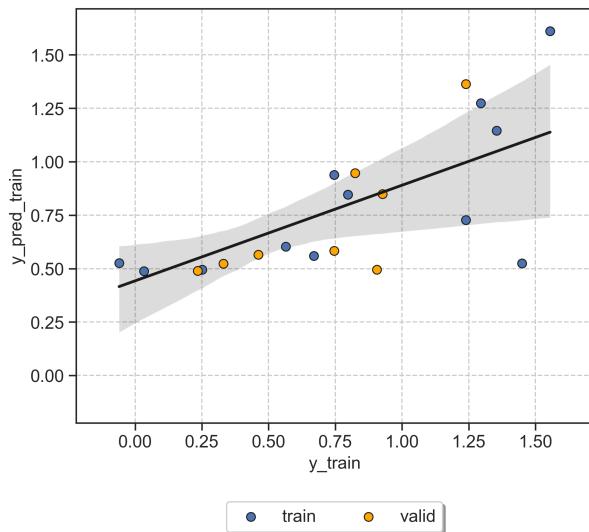
Predictions\_train\_valid of GB\_90\_PFI



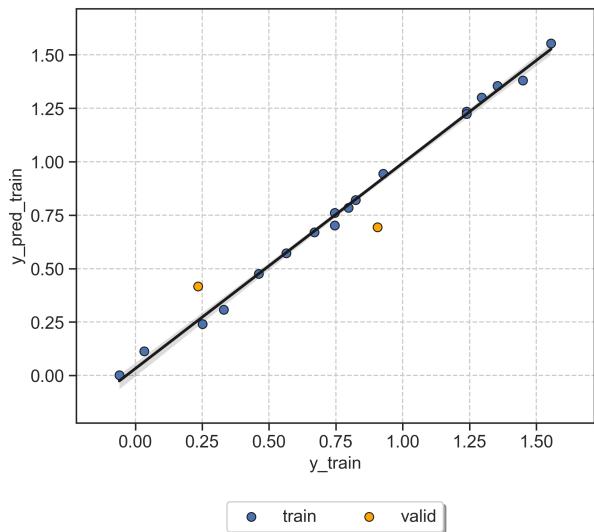
Predictions\_train\_valid of NN\_60\_No\_PFI



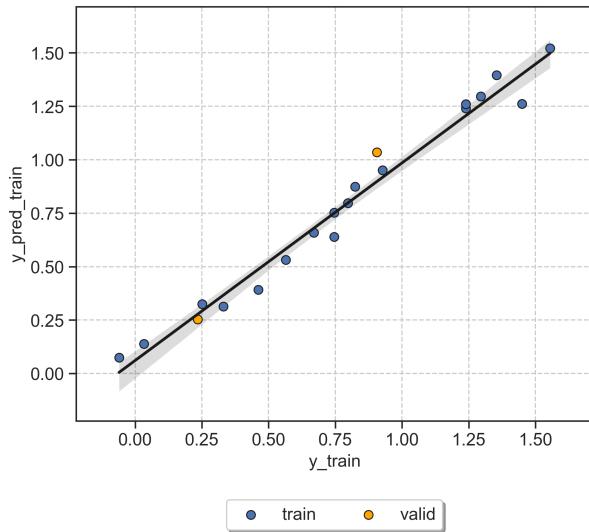
Predictions\_train\_valid of NN\_60\_PFI



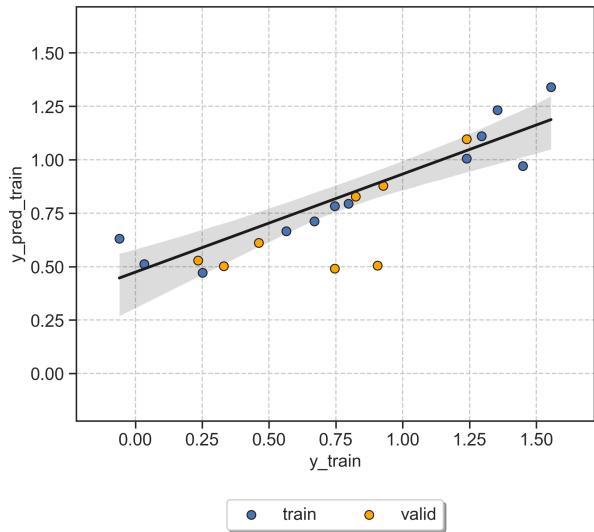
Predictions\_train\_valid of NN\_90\_No\_PFI

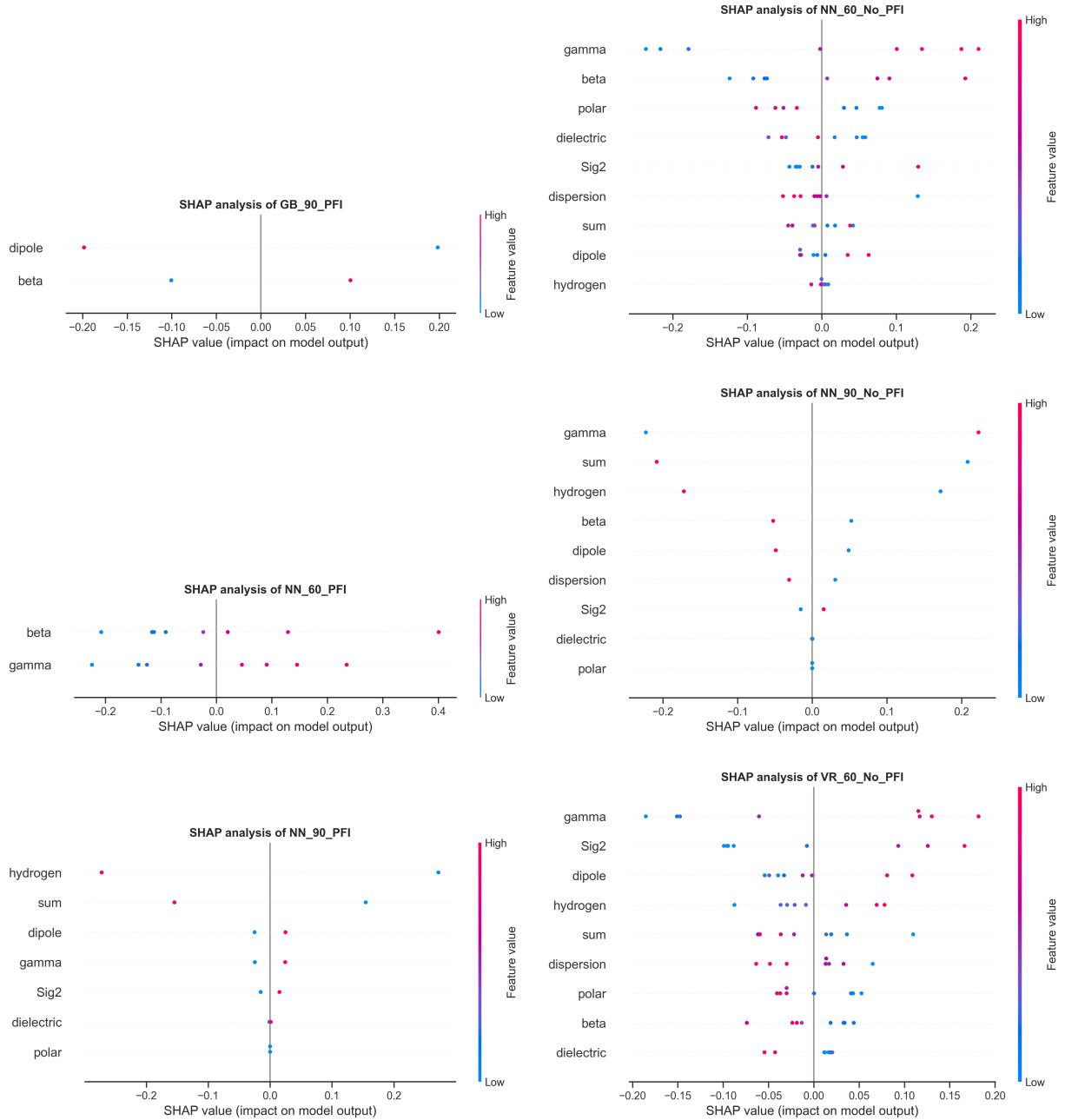


Predictions\_train\_valid of NN\_90\_PFI



Predictions\_train\_valid of VR\_60\_No\_PFI





- 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', 'hydrogen', 'sum', 'dipole', 'Sig2']
  - Training points: 12
  - Validation points: 8
- 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
- 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
- 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
  - o VERIFY donut plots saved in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\BandarVERIFY\VERIFY\_tests\_NN\_60\_No\_PFI.png
    - o VERIFY test values saved in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\BandarVERIFY\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\_test 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 were 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 were 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 were 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\Artículo ROBERT\Pruebas\_ROBERT\Regression\BandarVERIFY\VERIFY\_tests\_NN\_60\_PFI.png
    - o VERIFY test values saved in C:\Users\David\Desktop\Artículo ROBERT\Pruebas\_ROBERT\Regression\BandarVERIFY\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\_test 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

