Machine-learning models for λ and $\omega_{\log}$

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This notebook is a part of [Huan Tran & Tuoc N. Vu, *Machine-learning approach for discovery of conventional superconductors*, published in Phys. Rev. Materials **7**, 054805 (2023)], and is also an example of matsML toolkit. Results obtained here can be found in this work.

This notebook prodives two featurized datasets of λ and $\omega_{\log}$ and the scripts to train some machine-learning (ML) models reported in the Reference above. λ and $\omega_{\log}$ are two important parameters characterizing the electron-phonon interactions that can be used to compute the critical temperature T_c of a superconducting material in some simple ways, one of which is the McMillan equation [W. L. McMillan, Phys. Rev. **167**, 331 (1968)].

The raw datasets used for [Huan Tran & Tuoc N. Vu, *Machine-learning approach for discovery of conventional superconductors*] and in this notebook were curated from the scientific literature. They contains the materials atomic structures from which λ and $\omega_{\log}$ were computed using DFPT and reported, mostly in the 2010s and 2020s. Two fearurized datasets (data_lambda.csv and data_omlog.csv) that are provided here were prepared using Matminer and some feature engineering techniques.

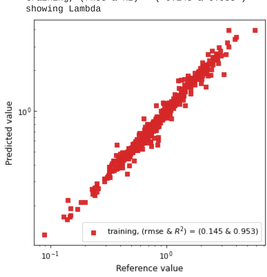
In [1]:
```
import os
import pandas as pd
```

Lambda data and training models

In [2]:
```
data_file = "data_lambda.csv"
id_col=['ind']                      # this is id column in the fingerprint data
y_cols=['lambda']                   # this is y columns
comment_cols=[]                     # other columns that are not id, not x, nor y columns

n_trains = 1.00                     # 100% for training, 0% for validating
sampling = 'random'                 # way of train/test spliting. Random, stratified
x_scaling='minmax'
y_scaling='logpos'

data_params = {'data_file': data_file, 'id_col':id_col, 'y_cols':y_cols,
               'comment_cols':comment_cols, 'y_scaling':y_scaling,
               'x_scaling':x_scaling, 'sampling':sampling, 'n_trains':n_trains}
```

In [3]:
```
from matsml.models import GPR

# Model parameters
nfold_cv = 5                        # Number of folds for cross validation
model_file = 'model_gpr.pkl'        # Name of the model file to be created
verbosity = 0
rmse_cv = False
n_restarts_optimizer = 0
kernel = 'Matern'                   # RBF, DotProduct, Matern
noise_lb = 0.0300
noise_ub = 100

model_params={'nfold_cv':nfold_cv,'model_file':model_file,'verbosity':verbosity,
              'n_restarts_optimizer':n_restarts_optimizer, 'rmse_cv':rmse_cv,
              'kernel': kernel, 'noise_lb':noise_lb, 'noise_ub':noise_ub}

model=GPR(data_params = data_params,model_params = model_params)
model.train()
model.plot(pdf_output=False)
```

```
 matsML, v1.3.0
 *****

 Checking parameters
   all passed                    True

 Learning fingerprinted/featured data
   algorithm                     gaussian process regression w/ scikit-learn
   kernel                        Matern
   nfold_cv                      5
   optimizer                     fmin_l_bfgs_b
   n_restarts_optimizer          0
   noise_lb                      0.03
   noise_ub                      100
   rmse_cv                       False
 Read data
   data file                     data_lambda.csv
   data size                     584
   training size                 100.0  %
   test size                     0.0  %
   x dimensionality              40
   y dimensionality              1
   y label(s)                    ['lambda']
 Scaling x                       minmax
   xscaler saved in              xscaler.pkl
 Scaling y                       logpos
 Prepare train/test sets         random
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.068966 0.312211 0.312211
   cv,rmse_train,rmse_test,rmse_opt: 1 0.085361 0.310039 0.310039
   cv,rmse_train,rmse_test,rmse_opt: 2 0.082541 0.277294 0.277294
   cv,rmse_train,rmse_test,rmse_opt: 3 0.093931 0.364798 0.277294
   cv,rmse_train,rmse_test,rmse_opt: 4 0.085187 0.503576 0.277294
 GPR model trained, now make predictions & invert scaling
   unscaling y: logpos
      rmse training      Lambda           0.144566
 Predictions made & saved in "training.csv"
 Plot results in "training.csv" & "test.csv"
   training, (rmse & R2) = ( 0.145 & 0.953 )
   showing Lambda
```



Omlog data and model training

In [4]:
```
data_file = 'data_omlog.csv'
id_col=['ind']                      # this is id column in the fingerprint data
y_cols=['omlog']                    # this is y columns
comment_cols=[]                     # other columns that are not id, not x, nor y columns

n_trains = 1.00                     # 100% for training, 0% for validating
sampling = 'random'                 # way of train/test spliting. Random, stratified
x_scaling='minmax'
y_scaling='minmax'

data_params = {'data_file': data_file, 'id_col': id_col,'y_cols': y_cols,
               'comment_cols': comment_cols,'y_scaling': y_scaling,
               'x_scaling': x_scaling, 'sampling': sampling, 'n_trains': n_trains}
```

In [5]:
```
from matsml.models import GPR

# Model parameters
nfold_cv = 5                        # Number of folds for cross validation
model_file = 'model_gpr.pkl'        # Name of the model file to be created
verbosity = 0
rmse_cv = False
n_restarts_optimizer = 3
kernel = 'Matern'                   # RBF, DotProduct, Matern
noise_lb = 0.0250
noise_ub = 100

model_params={'nfold_cv':nfold_cv,'model_file':model_file,'verbosity':verbosity,
              'n_restarts_optimizer':n_restarts_optimizer, 'rmse_cv':rmse_cv,
              'kernel': kernel, 'noise_lb':noise_lb, 'noise_ub':noise_ub}

model=GPR(data_params = data_params,model_params = model_params)
model.train()
model.plot(pdf_output=False)
```

```
 Checking parameters
   all passed                    True

 Learning fingerprinted/featured data
   algorithm                     gaussian process regression w/ scikit-learn
   kernel                        Matern
   nfold_cv                      5
   optimizer                     fmin_l_bfgs_b
   n_restarts_optimizer          3
   noise_lb                      0.025
   noise_ub                      100
   rmse_cv                       False
 Read data
   data file                     data_omlog.csv
   data size                     567
   training size                 100.0  %
   test size                     0.0  %
   x dimensionality              38
   y dimensionality              1
   y label(s)                    ['omlog']
 Scaling x                       minmax
   xscaler saved in              xscaler.pkl
 Scaling y                       minmax
 Prepare train/test sets         random
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.047413 0.088902 0.088902
   cv,rmse_train,rmse_test,rmse_opt: 1 0.049560 0.081160 0.081160
   cv,rmse_train,rmse_test,rmse_opt: 2 0.048238 0.094992 0.081160
   cv,rmse_train,rmse_test,rmse_opt: 3 0.052725 0.091205 0.081160
   cv,rmse_train,rmse_test,rmse_opt: 4 0.049675 0.096612 0.081160
 GPR model trained, now make predictions & invert scaling
   unscaling y: minmax
      rmse training      omlog            110.175303
 Predictions made & saved in "training.csv"
 Plot results in "training.csv" & "test.csv"
   training, (rmse & R2) = ( 110.175 & 0.943 )
   showing omlog
```