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

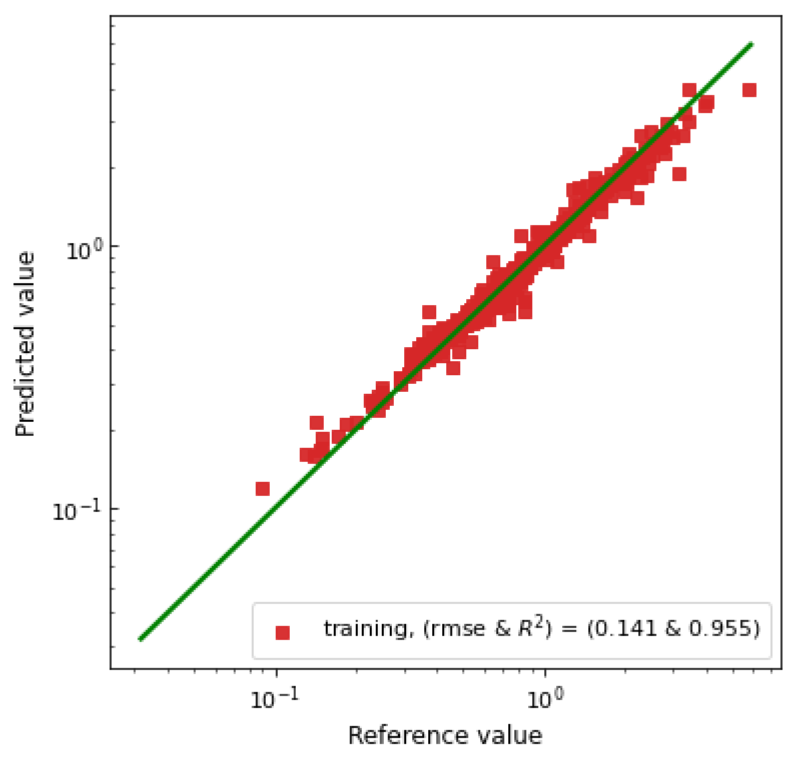
In [2]:

```
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

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 0.079945 0.360401 0.360401
  cv,rmse_train,rmse_test,rmse_opt: 1 0.080406 0.399396 0.360401
  cv,rmse_train,rmse_test,rmse_opt: 2 0.081069 0.337944 0.337944
  cv,rmse_train,rmse_test,rmse_opt: 3 0.086021 0.401213 0.337944
  cv,rmse_train,rmse_test,rmse_opt: 4 0.091352 0.377160 0.337944
GPR model trained, now make predictions & invert scaling
  unscaling y: logpos
     rmse training     Lambda           0.141403
Predictions made & saved in "training.csv"
Plot results in "training.csv" & "test.csv"
  training, (rmse & R2) = ( 0.141 & 0.955 )
  showing Lambda
```



Omlog data and model training

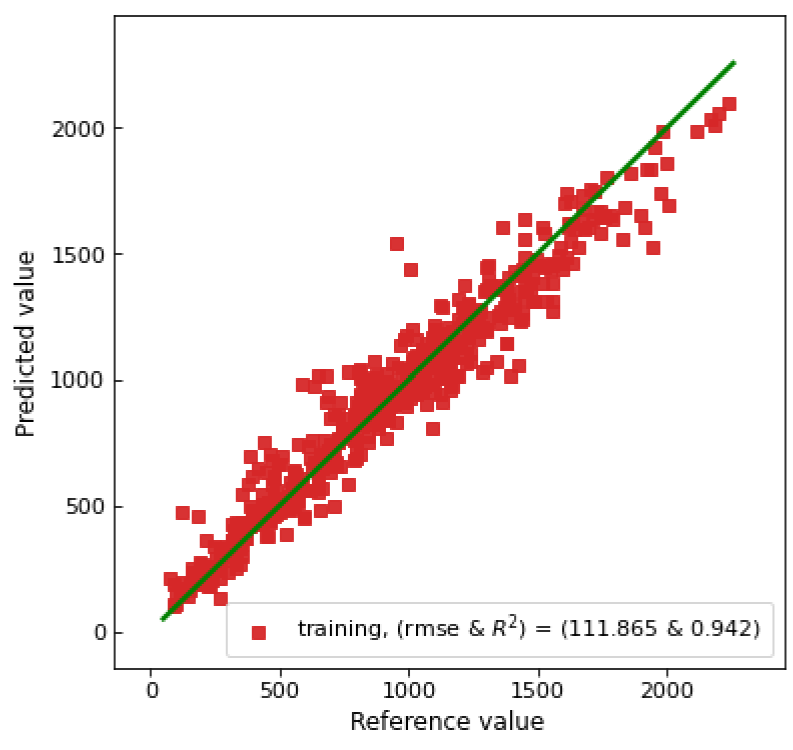
In [4]:

```
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 = 1.0                      # 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 0.047682 0.089167 0.089167
  cv,rmse_train,rmse_test,rmse_opt: 1 0.049713 0.091803 0.089167
  cv,rmse_train,rmse_test,rmse_opt: 2 0.051706 0.092974 0.089167
  cv,rmse_train,rmse_test,rmse_opt: 3 0.050107 0.095840 0.089167
  cv,rmse_train,rmse_test,rmse_opt: 4 0.049112 0.098038 0.089167
GPR model trained, now make predictions & invert scaling
  unscaling y: minmax
     rmse training     omlog            111.865368
Predictions made & saved in "training.csv"
Plot results in "training.csv" & "test.csv"
  training, (rmse & R2) = ( 111.865 & 0.942 )
  showing omlog
```



In [ ]: