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.

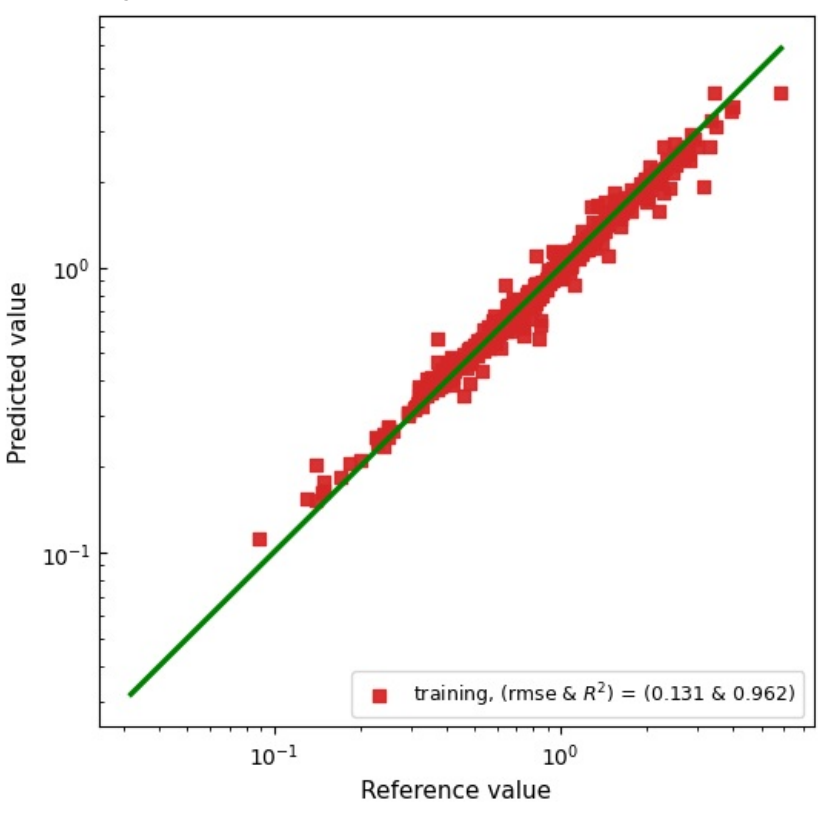
In [1]:
```
import os
import pandas as pd
```

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 column
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 splitting. 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 0.088892 0.341812 0.341812
    cv,rmse_train,rmse_test,rmse_opt: 1 0.096778 0.371475 0.341812
    cv,rmse_train,rmse_test,rmse_opt: 2 0.082219 0.348912 0.341812
    cv,rmse_train,rmse_test,rmse_opt: 3 0.083992 0.399081 0.341812
    cv,rmse_train,rmse_test,rmse_opt: 4 0.072759 0.397405 0.341812

  GPR model trained, now make predictions & invert scaling
    unscaling y: logpos
       rmse training     Lambda           0.130671

  Predictions made & saved in "training.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.131 & 0.962 )
    showing Lambda
```

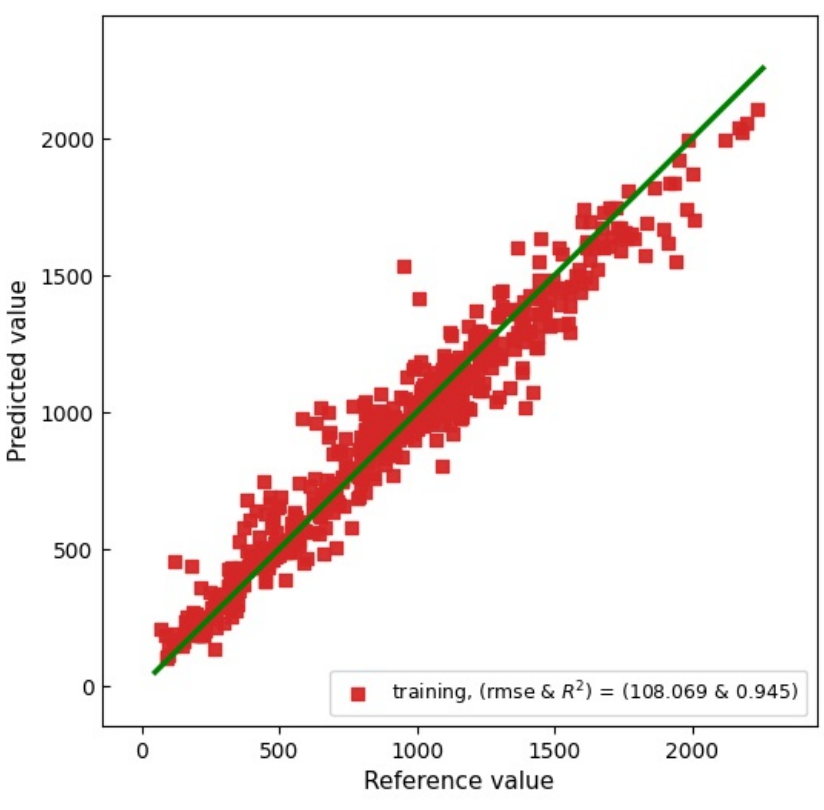


Omlog data and model training

In [4]:
```
data_file = 'data_omlog.csv'
id_col = ['ind']          # this is id column in the fingerprint data
y_cols = ['omlog']        # this is y column
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 splitting: 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 0.048147 0.084214 0.084214
    cv,rmse_train,rmse_test,rmse_opt: 1 0.049136 0.087246 0.084214
    cv,rmse_train,rmse_test,rmse_opt: 2 0.049198 0.081890 0.081890
    cv,rmse_train,rmse_test,rmse_opt: 3 0.051584 0.102325 0.081890
    cv,rmse_train,rmse_test,rmse_opt: 4 0.050620 0.088216 0.081890

  GPR model trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     omlog            108.069398

  Predictions made & saved in "training.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 108.069 & 0.945 )
    showing omlog
```



In [ ]: