Example 2: Fingerpring molecules data and learning energy

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The main objective of this example is to demonstrate a generic workflow of materials, involving (1) obtaining a small dataset of molecules and their energy, (2) fingerprint them, and (3) develop some ML models.

1. Download a dataset

The dataset contains 10,000 non-equilibrium structures of CH_3-NH-OH molecules, whose energy was computed using BigDFT package and HGH norm-conserving pseudopotentials. It is available at www.matsml.org.

In [1]:
```python
from matsml.data import Datasets
import pandas as pd
import os

# Load a dataset
dataset_name = 'molecs_CH3NHOH'
data = Datasets(dataset_name=dataset_name)
data.load_dataset()

# Have a look at the content
summary_path = os.path.join(os.getcwd(), str(dataset_name), 'summary.csv')
print(pd.read_csv(summary_path))
```

```
  matsML, v1.3.0
  *****
  Load requested dataset(s)
  Data saved in molecs_CH3NHOH
            file_name      target
0     CH3NHOH_00001.xyz -940.288539
1     CH3NHOH_00002.xyz -940.580380
2     CH3NHOH_00003.xyz -940.184809
3     CH3NHOH_00004.xyz -940.460977
4     CH3NHOH_00005.xyz -940.579457
...                 ...         ...
9994  CH3NHOH_09996.xyz -940.286083
9995  CH3NHOH_09997.xyz -940.744461
9996  CH3NHOH_09998.xyz -940.553979
9997  CH3NHOH_09999.xyz -940.650902
9998  CH3NHOH_10000.xyz -940.059079

[9999 rows x 2 columns]
```

2. Fingerprint the obtained data

Two kinds of fingerprints will be demonstrated here

1. Coulomb matrix (CM) [M. Rupp, A. Tkatchenko, K.-R. Müller, and O. Anatole von Lilienfeld, *Fast and accurate modeling of molecular atomization energies with machine learning*, Phys. Rev. Lett., 108, 058301 (2012)] is perhaps one of the earliest fingerprints used in materials informatics. It was defined as an $N \times N$ matrix for a molecule of N atoms. The key advantage of CM is that it is invariant under rotations and translations, required ro represent materials structure as a whole. However, its size depends on the molecule size, making it not directly usable for machine learning. Normally, the eigenvalues of these matricies are computed and sorted, and then zero padding is used to make fixed-size vectors. Here, we defined a projection of these Coulomb matricies onto a set of Gaussian functions, covering the entire range of the Coulomn matrix element values. The results are also a set of fixed-size fingerprints, which are ready for learning. Keyword for this fingerprint is **pcm_molecs**.

2. Smooth Overlap of Atomic Positions (SOAP) [S. De, A. P. Bartók, G. Csányi, and M. Ceriotti, *Comparing molecules and solids across structural and alchemical space*, Phys. Chem. Chem. Phys. **18**, 13754 (2016)] is a more sophisticated fingerprint. Keyword for this fingerprint is **soap_molecs**.

In [2]:
```python
from matsml.fingerprint import Fingerprint
import os

summary = os.path.join(os.getcwd(), 'molecs_CH3NHOH/summary.csv')
data_loc = os.path.join(os.getcwd(), 'molecs_CH3NHOH/')
fp_dim = 50                           # intended fingerprint dimensionality; the final number can be smaller
verbosity = 0                         # verbosity, 0 or 1

# PCM
data_params_pcm = {
    'fp_type': 'pcm_molecs',
    'summary': summary,
    'data_loc': data_loc,
    'fp_file': 'fp_pcm.csv',
    'fp_dim': fp_dim,
    'verbosity': verbosity
}

fp_pcm = Fingerprint(data_params_pcm)
fp_pcm.get_fingerprint()

# SOAP
data_params_soap = {
    'fp_type': 'soap_molecs',
    'summary': summary,
    'data_loc': data_loc,
    'fp_file': 'fp_soap.csv',
    'fp_dim': fp_dim,
    'verbosity': verbosity
}

fp_soap = Fingerprint(data_params_soap)
fp_soap.get_fingerprint()
```

```
  Atomic structure fingerprinting
    summary                     /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH3NHOH/summary.cs
v
    data_loc                    /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH3NHOH/
    fp_type                     pcm_molecs
    fp_file                     fp_pcm.csv
    fp_dim                      50
    verbosity                   0
  Read input
    num_structs                 9999
  Computing Coulomb matrix
    [==================================================] 100%
  Projecting Coulomb matrix to create fingerprints
    [==================================================] 100%
  Done fingerprinting, results saved in fp_pcm.csv
  Atomic structure fingerprinting
    summary                     /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH3NHOH/summary.cs
v
    data_loc                    /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH3NHOH/
    fp_type                     soap_molecs
    fp_file                     fp_soap.csv
    fp_dim                      50
    verbosity                   0
  Read input
    num_structs                 9999
  Computing SOAP fingerprint with DScribe
    [==================================================] 100%
  Done fingerprinting, results saved in fp_soap.csv
```

The fingerprinting step is slow. A version of fingerprinted data can also be obtained in case you want to skip this step. Pandas can read gzip files fo no need to unzip them.

In [3]:
```python
from matsml.data import Datasets
import os

# Load data
data = Datasets(ds1='fp_molecs_CH3NHOH_pcm', ds2='fp_molecs_CH3NHOH_soap')
data.load_dataset()

print(os.path.isfile('fp_molecs_CH3NHOH_pcm.csv.gz'))
print(os.path.isfile('fp_molecs_CH3NHOH_soap.csv.gz'))
```

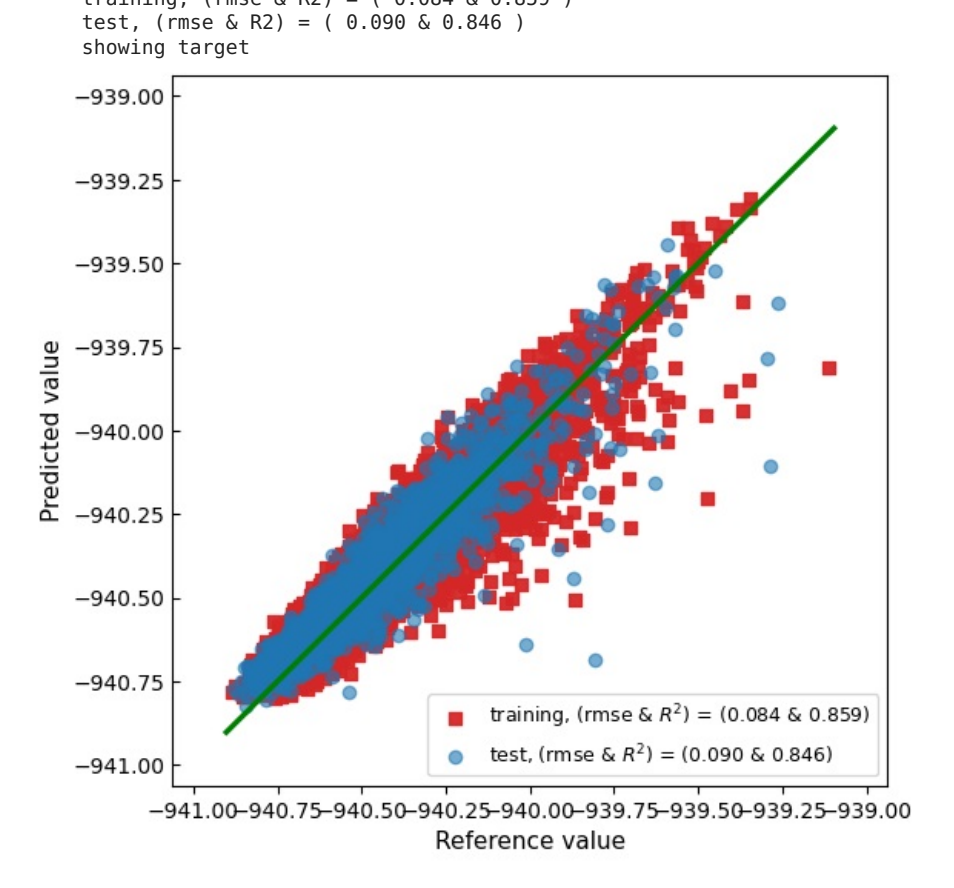
```
  Load requested dataset(s)
  Data saved in fp_molecs_CH3NHOH_pcm.csv.gz
  Data saved in fp_molecs_CH3NHOH_soap.csv.gz
True
True
```

3. Train some ML models with "fp_pcm.csv" and "fp_soap.csv" just created

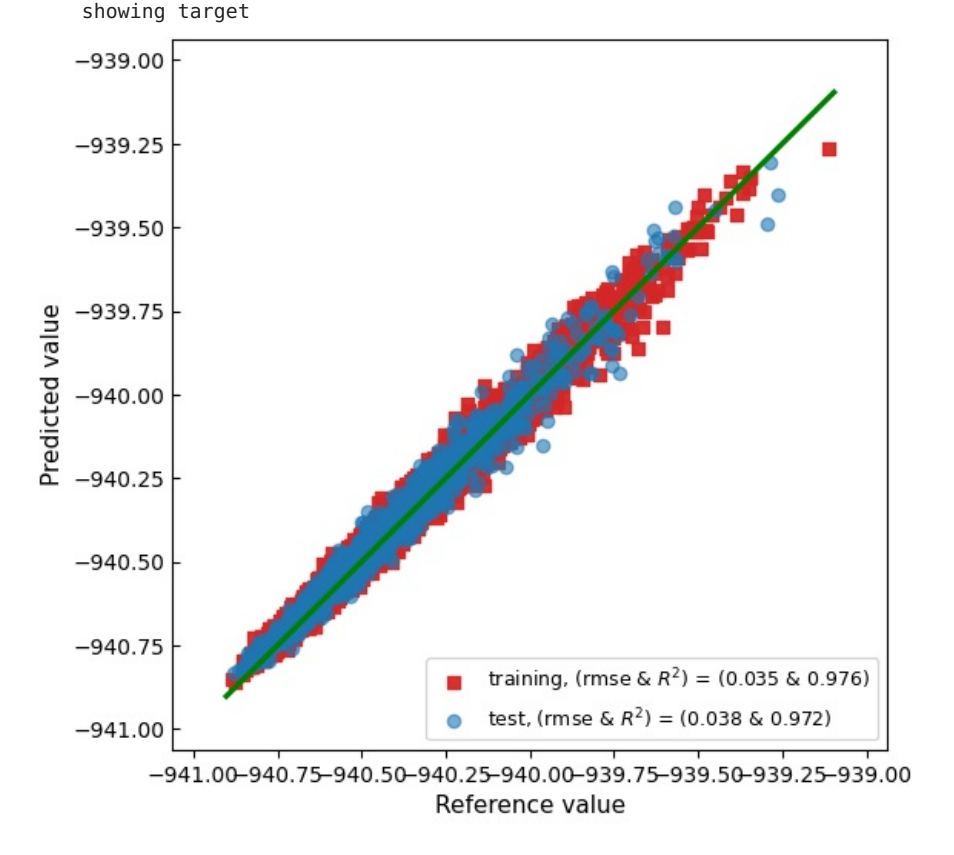
In [4]:
```python
# data parameters for learning

id_col = ['id']              # column for data ID
y_cols = ['target']          # columns for (one or more) target properties
comment_cols = []            # comment columns, anything not counted into ID, fingerprints, and target
n_trains = 0.8               # 80% for training, 20% for validating
sampling = 'random'          # method for train/test splitting
x_scaling = 'minmax'         # method for x scaling
y_scaling = 'minmax'         # method for y scaling

# Dict of data parameters
data_params_pcm = {
    'data_file': 'fp_molecs_CH3NHOH_pcm.csv.gz',
    '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
}

data_params_soap = {
    'data_file': 'fp_molecs_CH3NHOH_soap.csv.gz',
    '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]:
```python
from matsml.models import FCNN

# Model parameters
layers = [8, 8, 8]              # list of nodes in hidden layers
epochs = 200                    # Epochs
nfold_cv = 5                    # Number of folds for cross validation
use_bias = True                # Use bias term or not
model_file = 'model_nn.pkl'    # Name of the model file to be created
verbosity = 0                  # Verbosity, 0 or 1
batch_size = 32                # Default = 32
loss = 'mse'
activ_funct = 'selu'           # Options: "tanh", "relu", and more
optimizer = 'nadam'            # Options: "Nadam", "Adam", and more

# Dict of model parameters
model_params = {
    'layers': layers,
    'activ_funct': activ_funct,
    'epochs': epochs,
    'nfold_cv': nfold_cv,
    'optimizer': optimizer,
    'use_bias': use_bias,
    'model_file': model_file,
    'loss': loss,
    'batch_size': batch_size,
    'verbosity': verbosity,
    'rmse_cv': False
}

# PCM
model = FCNN(data_params=data_params_pcm, model_params=model_params)
model.train()
model.plot(pdf_output=False)

# SOAP
model = FCNN(data_params=data_params_soap, model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
  Checking parameters
    model_file not ends with ".weights.h5", renamed

  Learning fingerprinted/featured data
    algorithm                   fully connected NeuralNet w/ TensorFlow
    layers                      [8, 8, 8]
    activ_funct                 selu
    epochs                      200
    optimizer                   nadam
    nfold_cv                    5
    verbosity                   0

  Read data
    data file                   fp_molecs_CH3NHOH_pcm.csv.gz
    data size                   9999
    training size               80.0  %
    test size                   20.0  %
    x dimensionality            38
    y dimensionality            1
    y label(s)                  ['target']

  Scaling x                     minmax
    xscaler saved in            xscaler.pkl

  Scaling y                     minmax

  Prepare train/test sets       random

  Building model                FCNN
WARNING: All log messages before absl::InitializeLog() is called are written to STDERR
I0000 00:00:1765080410.754694 1029906 gpu_device.cc:2020] Created device /job:localhost/replica:0/task:0/device
:GPU:0 with 4598 MB memory:  -> device: 0, name: NVIDIA GeForce RTX 2060, pci bus id: 0000:01:00.0, compute cap
ability: 7.5
  Training model w/ cross validation
I0000 00:00:1765080411.467892 1030088 device_compiler.h:196] Compiled cluster using XLA!  This line is logged a
t most once for the lifetime of the process.
200/200 [==============================] - 0s 359us/step
50/50 [==============================] - 0s 374us/step
    cv,rmse_train,rmse_test,rmse_opt: 0 0.050092 0.049035 0.049035
200/200 [==============================] - 0s 367us/step
50/50 [==============================] - 0s 363us/step
    cv,rmse_train,rmse_test,rmse_opt: 1 0.046076 0.048751 0.048751
200/200 [==============================] - 0s 397us/step
50/50 [==============================] - 0s 376us/step
    cv,rmse_train,rmse_test,rmse_opt: 2 0.045175 0.048834 0.048751
200/200 [==============================] - 0s 360us/step
50/50 [==============================] - 0s 359us/step
    cv,rmse_train,rmse_test,rmse_opt: 3 0.047309 0.048480 0.048480
200/200 [==============================] - 0s 365us/step
50/50 [==============================] - 0s 362us/step
    cv,rmse_train,rmse_test,rmse_opt: 4 0.047316 0.049786 0.048480
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
250/250 [==============================] - 0s 418us/step
    unscaling y: minmax
       rmse training     target           0.084167
63/63 [==============================] - 0s 401us/step
    unscaling y: minmax
       rmse test         target           0.089707
  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.084 & 0.859 )
    test, (rmse & R2) = ( 0.090 & 0.846 )
    showing target
```



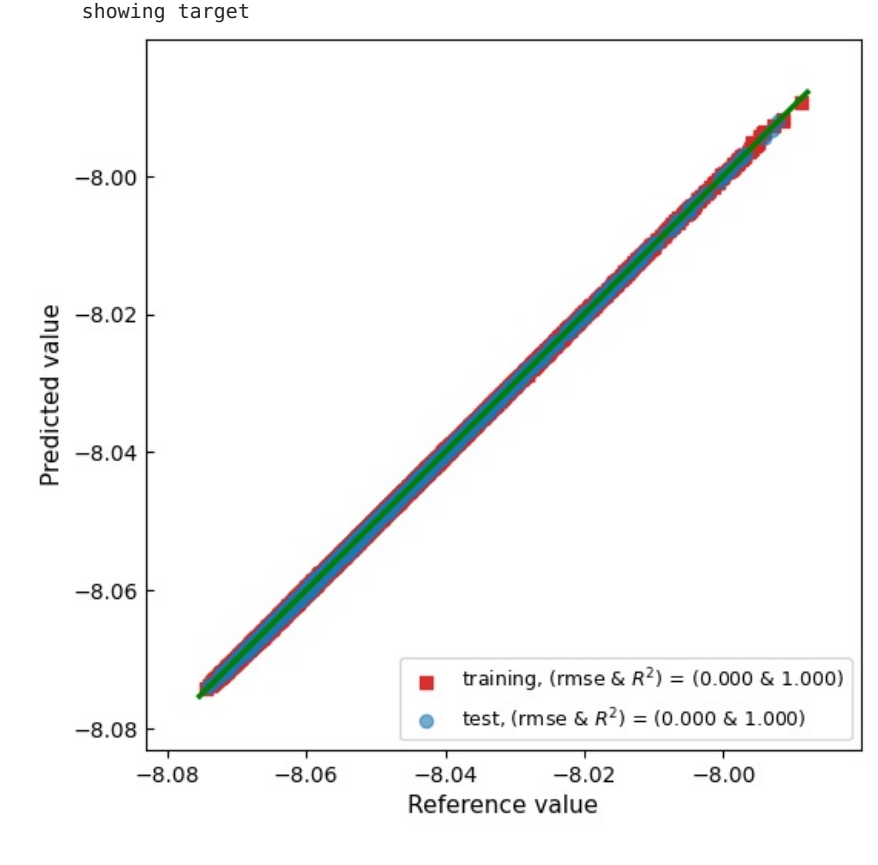

```
  Checking parameters
    model_file not ends with ".weights.h5", renamed

  Learning fingerprinted/featured data
    algorithm                   fully connected NeuralNet w/ TensorFlow
    layers                      [8, 8, 8]
    activ_funct                 selu
    epochs                      200
    optimizer                   nadam
    nfold_cv                    5
    verbosity                   0

  Read data
    data file                   fp_molecs_CH3NHOH_soap.csv.gz
    data size                   9999
    training size               80.0  %
    test size                   20.0  %
    x dimensionality            220
    y dimensionality            1
    y label(s)                  ['target']

  Scaling x                     minmax
    xscaler saved in            xscaler.pkl

  Scaling y                     minmax

  Prepare train/test sets       random

  Building model                FCNN
  Training model w/ cross validation
200/200 [==============================] - 0s 446us/step
50/50 [==============================] - 0s 427us/step
    cv,rmse_train,rmse_test,rmse_opt: 0 0.026899 0.028037 0.028037
200/200 [==============================] - 0s 433us/step
50/50 [==============================] - 0s 424us/step
    cv,rmse_train,rmse_test,rmse_opt: 1 0.021439 0.022892 0.022892
200/200 [==============================] - 0s 431us/step
50/50 [==============================] - 0s 427us/step
    cv,rmse_train,rmse_test,rmse_opt: 2 0.022278 0.022738 0.022738
200/200 [==============================] - 0s 440us/step
50/50 [==============================] - 0s 437us/step
    cv,rmse_train,rmse_test,rmse_opt: 3 0.023362 0.024705 0.022738
200/200 [==============================] - 0s 427us/step
50/50 [==============================] - 0s 476us/step
    cv,rmse_train,rmse_test,rmse_opt: 4 0.019324 0.020762 0.020762
    Optimal ncv:  4 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
250/250 [==============================] - 0s 458us/step
    unscaling y: minmax
       rmse training     target           0.034732
63/63 [==============================] - 0s 427us/step
    unscaling y: minmax
       rmse test         target           0.038098
  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.035 & 0.976 )
    test, (rmse & R2) = ( 0.038 & 0.972 )
    showing target
```



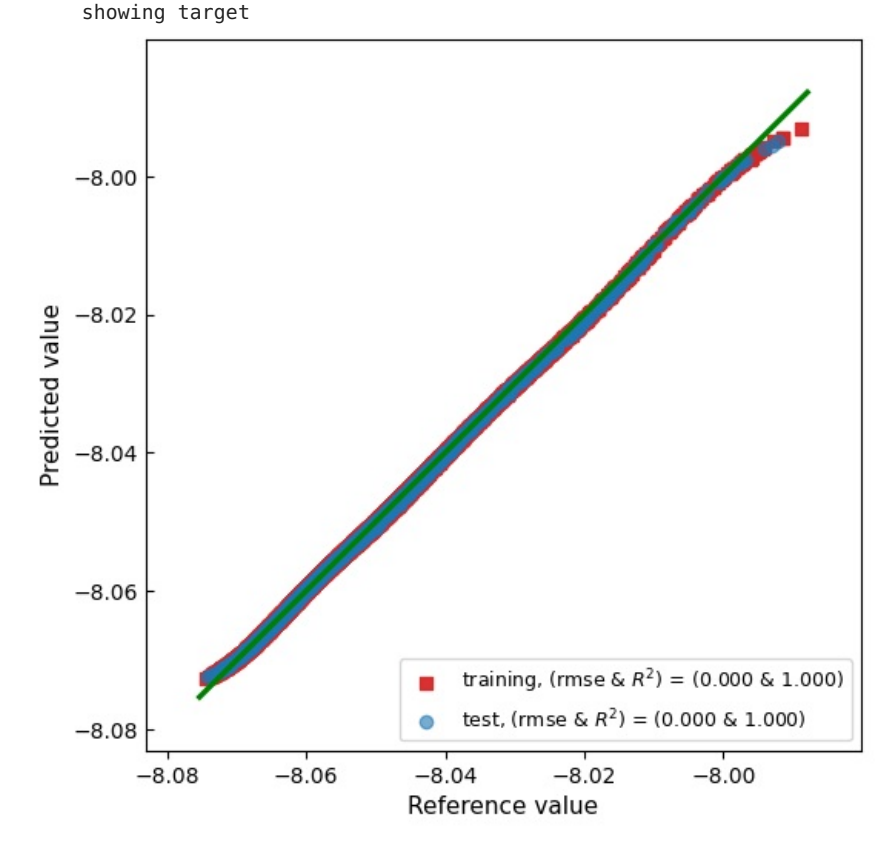
4. The same flowwork with the CH_4 dataset

In [6]:
```python
# Load data
from matsml.data import Datasets
import pandas as pd
import os

data = Datasets(dataset_name='molecs_CH4')
data.load_dataset()
print(pd.read_csv('molecs_CH4/summary.csv'))

# Fingerprint
from matsml.fingerprint import Fingerprint

summary = os.path.join(os.getcwd(), 'molecs_CH4/summary.csv')
data_loc = os.path.join(os.getcwd(), 'molecs_CH4/')
fp_type = 'pcm_molecs'                   # projected Coulomb matrix for molecules
fp_dim = 100                             # intended fingerprint dimensionality; the final number can be smaller
verbosity = 0                            # verbosity, 0 or 1

# PCM
data_params_pcm = {
    'fp_type': 'pcm_molecs',
    'summary': summary,
    'data_loc': data_loc,
    'fp_file': 'fp_CH4_pcm.csv',
    'fp_dim': fp_dim,
    'verbosity': verbosity
}

fp_pcm = Fingerprint(data_params_pcm)
fp_pcm.get_fingerprint()

# SOAP
data_params_soap = {
    'fp_type': 'soap_molecs',
    'summary': summary,
    'data_loc': data_loc,
    'fp_file': 'fp_CH4_soap.csv',
    'fp_dim': fp_dim,
    'verbosity': verbosity
}

fp_soap = Fingerprint(data_params_soap)
fp_soap.get_fingerprint()

# Data params
id_col = ['id']              # column for data ID
y_cols = ['target']          # target property column(s)
comment_cols = []            # comment columns
n_trains = 0.8               # 80% training, 20% validation
sampling = 'random'          # train/test split method
x_scaling = 'minmax'         # x scaling method
y_scaling = 'minmax'         # y scaling method

# Dict of data parameters
data_params_CH4_pcm = {
    'data_file': 'fp_CH4_pcm.csv',
    '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
}

data_params_CH4_soap = {
    'data_file': 'fp_CH4_soap.csv',
    '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
}

# Models with FCNN
from matsml.models import FCNN

# Model parameters
layers = [4, 4]                # hidden layer sizes
epochs = 200                   # training epochs
nfold_cv = 5                   # cross-validation folds
use_bias = True                # use bias term
model_file = 'model_nn.pkl'    # model output file
verbosity = 0                  # verbosity level
batch_size = 32                # batch size
loss = 'mse'
activ_funct = 'tanh'           # activation function
optimizer = 'nadam'            # optimizer

# Dict of model parameters
model_params = {
    'layers': layers,
    'activ_funct': activ_funct,
    'epochs': epochs,
    'nfold_cv': nfold_cv,
    'optimizer': optimizer,
    'use_bias': use_bias,
    'model_file': model_file,
    'loss': loss,
    'batch_size': batch_size,
    'verbosity': verbosity,
    'rmse_cv': False
}

# PCM Model
model = FCNN(data_params=data_params_CH4_pcm, model_params=model_params)
model.train()
model.plot(pdf_output=False)

# SOAP Model
model = FCNN(data_params=data_params_CH4_soap, model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
  Load requested dataset(s)
  Data saved in molecs_CH4
          file_name    target
0     CH4-00001.xyz -8.067843
1     CH4-00002.xyz -8.052410
2     CH4-00003.xyz -8.062879
3     CH4-00004.xyz -8.053809
4     CH4-00005.xyz -8.054724
...             ...       ...
9995  CH4-09996.xyz -8.061287
9996  CH4-09997.xyz -8.060672
9997  CH4-09998.xyz -8.013882
9998  CH4-09999.xyz -8.054027
9999  CH4-10000.xyz -8.052808

[10000 rows x 2 columns]
  Atomic structure fingerprinting
    summary                     /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH4/summary.csv
    data_loc                    /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH4/
    fp_type                     pcm_molecs
    fp_file                     fp_CH4_pcm.csv
    fp_dim                      100
    verbosity                   0
  Read input
    num_structs                 10000
  Computing Coulomb matrix
    [==================================================] 100%
  Projecting Coulomb matrix to create fingerprints
    [==================================================] 100%
  Done fingerprinting, results saved in fp_CH4_pcm.csv
  Atomic structure fingerprinting
    summary                     /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH4/summary.csv
    data_loc                    /home/huantran/work_local/matsml/examples/ex2_molecs/molecs_CH4/
    fp_type                     soap_molecs
    fp_file                     fp_CH4_soap.csv
    fp_dim                      100
    verbosity                   0
  Read input
    num_structs                 10000
  Computing SOAP fingerprint with DScribe
    [==================================================] 100%
  Done fingerprinting, results saved in fp_CH4_soap.csv

  Checking parameters
    model_file not ends with ".weights.h5", renamed

  Learning fingerprinted/featured data
    algorithm                   fully connected NeuralNet w/ TensorFlow
    layers                      [4, 4]
    activ_funct                 tanh
    epochs                      200
    optimizer                   nadam
    nfold_cv                    5
    verbosity                   0

  Read data
    data file                   fp_CH4_pcm.csv
    data size                   10000
    training size               80.0  %
    test size                   20.0  %
    x dimensionality            36
    y dimensionality            1
    y label(s)                  ['target']

  Scaling x                     minmax
    xscaler saved in            xscaler.pkl

  Scaling y                     minmax

  Prepare train/test sets       random

  Building model                FCNN
  Training model w/ cross validation
200/200 [==============================] - 0s 381us/step
50/50 [==============================] - 0s 405us/step
    cv,rmse_train,rmse_test,rmse_opt: 0 0.001706 0.001742 0.001742
200/200 [==============================] - 0s 384us/step
50/50 [==============================] - 0s 354us/step
    cv,rmse_train,rmse_test,rmse_opt: 1 0.001526 0.001501 0.001501
200/200 [==============================] - 0s 349us/step
50/50 [==============================] - 0s 344us/step
    cv,rmse_train,rmse_test,rmse_opt: 2 0.002794 0.002732 0.001501
200/200 [==============================] - 0s 410us/step
50/50 [==============================] - 0s 388us/step
    cv,rmse_train,rmse_test,rmse_opt: 3 0.001449 0.001521 0.001501
200/200 [==============================] - 0s 406us/step
50/50 [==============================] - 0s 400us/step
    cv,rmse_train,rmse_test,rmse_opt: 4 0.001867 0.001864 0.001501
    Optimal ncv:  1 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
250/250 [==============================] - 0s 387us/step
    unscaling y: minmax
       rmse training     target           0.00013
63/63 [==============================] - 0s 405us/step
    unscaling y: minmax
       rmse test         target           0.00013
  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.000 & 1.000 )
    test, (rmse & R2) = ( 0.000 & 1.000 )
    showing target
```




```
  Checking parameters
    model_file not ends with ".weights.h5", renamed

  Learning fingerprinted/featured data
    algorithm                   fully connected NeuralNet w/ TensorFlow
    layers                      [4, 4]
    activ_funct                 tanh
    epochs                      200
    optimizer                   nadam
    nfold_cv                    5
    verbosity                   0

  Read data
    data file                   fp_CH4_soap.csv
    data size                   10000
    training size               80.0  %
    test size                   20.0  %
    x dimensionality            735
    y dimensionality            1
    y label(s)                  ['target']

  Scaling x                     minmax
    xscaler saved in            xscaler.pkl

  Scaling y                     minmax

  Prepare train/test sets       random

  Building model                FCNN
  Training model w/ cross validation
200/200 [==============================] - 0s 420us/step
50/50 [==============================] - 0s 407us/step
    cv,rmse_train,rmse_test,rmse_opt: 0 0.004526 0.004760 0.004760
200/200 [==============================] - 0s 412us/step
50/50 [==============================] - 0s 413us/step
    cv,rmse_train,rmse_test,rmse_opt: 1 0.009737 0.009844 0.004760
200/200 [==============================] - 0s 408us/step
50/50 [==============================] - 0s 414us/step
    cv,rmse_train,rmse_test,rmse_opt: 2 0.003675 0.003673 0.003673
200/200 [==============================] - 0s 400us/step
50/50 [==============================] - 0s 405us/step
    cv,rmse_train,rmse_test,rmse_opt: 3 0.005457 0.005559 0.003673
200/200 [==============================] - 0s 420us/step
50/50 [==============================] - 0s 435us/step
    cv,rmse_train,rmse_test,rmse_opt: 4 0.003445 0.003299 0.003299
    Optimal ncv:  4 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
250/250 [==============================] - 0s 476us/step
    unscaling y: minmax
       rmse training     target           0.000293
63/63 [==============================] - 0s 2ms/step
    unscaling y: minmax
       rmse test         target           0.000287
  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.000 & 1.000 )
    test, (rmse & R2) = ( 0.000 & 1.000 )
    showing target
```



In [ ]: