Example 1: A quick look at 5 deterministic machine-learning models

Huan Tran

Some deterministic (non-probabilistic) ML models supported by matsML are introduced here. They models are

1. Support Vector Regression
2. Random Forest Regression
3. Kernel Ridge Regression
4. Gaussian Process Regression
5. Fully-Connected Neural Net

A simple dataset will be obtained from www.matsml.org for this example.

Load data

This is a *fingerprinted* dataset, being ready for machine learning. It contains 192 compositions of hybrid organic-inorganic perovskites, each of them is represented by a fingerprint vector and the averaged band gap of multiple atomic structures predicted for this composition. This dataset was used in *Probabilistic deep learning approach for targeted hybrid organic-inorganic perovskites*, Physical Review Materials **5**, 125402 (2021), and the raw data leading to this dataset is available at *A hybrid organic-inorganic perovskite dataset*, Scientific Data **4**, 170057 (2017).

In [1]:

```
from matsml.data import Datasets
import pandas as pd

# obtain data
data=Datasets(S1='fp_hoips_S1_1dest')
data.load_dataset()

# Have a look at the data fields. You will see "ID" is for the identification of the data points,
# 'Ymean' is the target (the averaged band gap mentioned above), and the others are the components
# of the fingerprint vector
fp_data = pd.read_csv('fp_hoips_S1_1dest.csv.gz')
print (fp_data.shape)
print (fp_data.columns)
```

```
  matsML, v1.3.0
  *****
  Load requested dataset(s)
  Data saved in fp_hoips_S1_1dest.csv.gz
(192, 34)
Index(['Unnamed: 0', 'ID', 'Ymean', 'MagpieData avg_dev GSvolume_pa',
       'MatscholarElementData mean embedding 54',
       'MatscholarElementData std_dev embedding 116',
       'MatscholarElementData std_dev embedding 155',
       'MatscholarElementData mean embedding 4',
       'PymatgenData mean mendeleev_no',
       'MatscholarElementData std_dev embedding 136',
       'MatscholarElementData std_dev embedding 153',
       'MatscholarElementData mean embedding 140',
       'MatscholarElementData mean embedding 170', 'H1N4H1', 'H1N3H1',
       'H1N3C3', 'N3C3N3', 'N3C3H1', 'H1C3C3', 'C3C3N3', 'C3N3C3', 'H1C4H1',
       'H1C4C4', 'C4C4C4', 'C4C4N4', 'H1C4N4', 'C4N4H1', 'N4N3H1', 'H1N4N3',
       'C4N4C4', 'H1N4O2', 'N4O2H1', 'C3C4H1', 'C4C3N3'],
      dtype='object')
```

Essential parameters of the obtained dataset, given as a dict, and needed for ML models

In [2]:

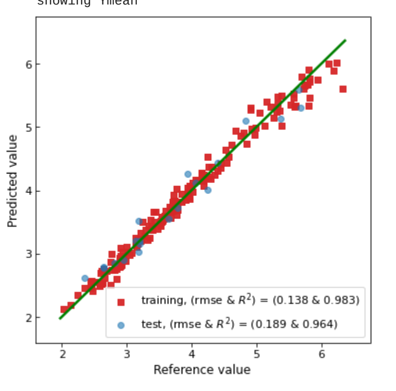
```
# data parameters
data_file ='fp_hoips_S1_1dest.csv.gz'
id_col = ['ID']
y_cols = ['Ymean']
comment_cols = []
n_trains = 0.9

sampling = 'random'
x_scaling = 'minmax'
y_scaling = 'normalize'

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}
```

Model 1: Support Vector Regression

In [3]:

```
from matsml.models import SVecR

# Model parameters
nfold_cv = 5
model_file = 'model_svr.pkl'
verbosity = 0
rmse_cv = False
regular_param = 2
kernel = 'rbf'
max_iter = -1

model_params = {'kernel': kernel,'nfold_cv': nfold_cv,'regular_param': regular_param,
                'max_iter': max_iter, 'model_file': model_file,'verbosity': verbosity,
                'rmse_cv':rmse_cv}

model = SVecR(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                   support vector regression w/ scikit-learn
    kernel                      rbf
    regular_param               2
    max_iter                    -1
    nfold_cv                    5
  Read data
    data file                   fp_hoips_S1_1dest.csv.gz
    data size                   192
    training size               89.6  %
    test size                   10.4  %
    x dimensionality            32
    y dimensionality            1
    y label(s)                  ['Ymean']
  Scaling x                     minmax
    xscaler saved in            xscaler.pkl
  Scaling y                     normalize
  Prepare train/test sets       random
  Training model w/ cross validation
    cv,rmse_train,rmse_test,rmse_opt: 0 0.122770 0.242234 0.242234
    cv,rmse_train,rmse_test,rmse_opt: 1 0.126141 0.174682 0.174682
    cv,rmse_train,rmse_test,rmse_opt: 2 0.123514 0.155424 0.155424
    cv,rmse_train,rmse_test,rmse_opt: 3 0.126768 0.155287 0.155287
    cv,rmse_train,rmse_test,rmse_opt: 4 0.123246 0.273079 0.155287
  RFR model trained and saved in "model_svr.pkl"
  Now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.138291
    unscaling y: normalize
       rmse test         Ymean            0.188509
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.138 & 0.983 )
    test, (rmse & R2) = ( 0.189 & 0.964 )
    showing Ymean
```

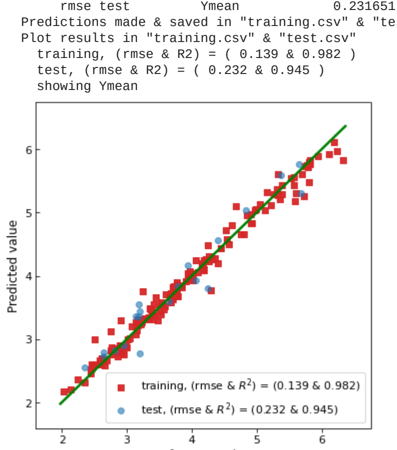


Model 2: Random Forest Regression

In [4]:

```
from matsml.models import RFR

# Model parameters
nfold_cv = 5
model_file = 'model_rfr.pkl'
verbosity = 0
rmse_cv = False
n_estimators = 20
random_state = 11
criterion = 'mse'
max_depth = 8
get_feature_importances = True

model_params = {'nfold_cv': nfold_cv, 'n_estimators': n_estimators, 'random_state': random_state,
                'criterion': criterion, 'max_depth': max_depth,
                'get_feature_importances': get_feature_importances, 'model_file': model_file,
                'verbosity': verbosity, 'rmse_cv': rmse_cv}

model = RFR(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                   random forest regression w/ scikit-learn
    nfold_cv                    5
    n_estimators                20
    max_depth                   8
    criterion                   mse
    get_feature_importances     True
    random_state                11
  Read data
    data file                   fp_hoips_S1_1dest.csv.gz
    data size                   192
    training size               89.6  %
    test size                   10.4  %
    x dimensionality            32
    y dimensionality            1
    y label(s)                  ['Ymean']
  Scaling x                     minmax
    xscaler saved in            xscaler.pkl
  Scaling y                     normalize
  Prepare train/test sets       random
  Training model w/ cross validation
    cv,rmse_train,rmse_test,rmse_opt: 0 0.083833 0.246096 0.246096
    cv,rmse_train,rmse_test,rmse_opt: 1 0.145150 0.074861 0.074861
    cv,rmse_train,rmse_test,rmse_opt: 2 0.143115 0.086780 0.074861
    cv,rmse_train,rmse_test,rmse_opt: 3 0.140634 0.101921 0.074861
    cv,rmse_train,rmse_test,rmse_opt: 4 0.145590 0.068049 0.068049
  RFR model trained and saved in "model_rfr.pkl"
  Top 10 features by importance
    MagpieData avg_dev GSvolume_pa                    importance: 0.451
    MatscholarElementData mean embedding 54           importance: 0.118
    MatscholarElementData mean embedding 4            importance: 0.111
    MatscholarElementData std_dev embedding 136       importance: 0.105
    MatscholarElementData mean embedding 170          importance: 0.055
    MatscholarElementData std_dev embedding 116       importance: 0.044
    MatscholarElementData std_dev embedding 155       importance: 0.044
    MatscholarElementData std_dev embedding 153       importance: 0.035
    MatscholarElementData mean embedding 140          importance: 0.025
    PymatgenData mean mendeleev_no                    importance: 0.004
  Now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.139311
    unscaling y: normalize
       rmse test         Ymean            0.231651
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.139 & 0.982 )
    test, (rmse & R2) = ( 0.232 & 0.945 )
    showing Ymean
```

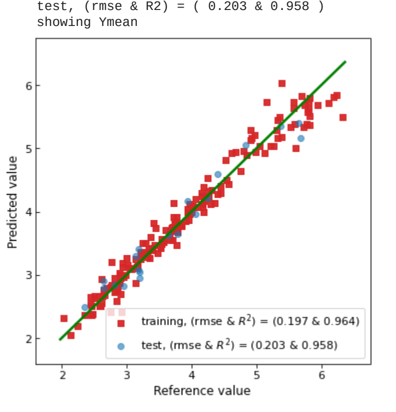


Model 3: Kernel Ridge Regression (KRR)

In [5]:

```
from matsml.models import KRR

# Model parameters
nfold_cv = 5
model_file = 'model_krr.pkl'
alpha = [-2,5]
gamma = [-2,5]
n_grids = 10
kernel = 'rbf'

model_params={'kernel': kernel, 'nfold_cv': nfold_cv, 'model_file': model_file, 'alpha': alpha,
              'gamma': gamma, 'n_grids': n_grids}

model = KRR(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                   kernel ridge regression w/ scikit-learn
    kernel                      rbf
    nfold_cv                    5
    alpha                       [-2, 5]
    gamma                       [-2, 5]
    number of alpha/gamma grids  10
  Read data
    data file                   fp_hoips_S1_1dest.csv.gz
    data size                   192
    training size               89.6  %
    test size                   10.4  %
    x dimensionality            32
    y dimensionality            1
    y label(s)                  ['Ymean']
  Scaling x                     minmax
    xscaler saved in            xscaler.pkl
  Scaling y                     normalize
  Prepare train/test sets       random
  Building model                KRR
  Training model w/ cross validation
  KRR model trained, now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.197196
    unscaling y: normalize
       rmse test         Ymean            0.202594
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.197 & 0.964 )
    test, (rmse & R2) = ( 0.203 & 0.958 )
    showing Ymean
```

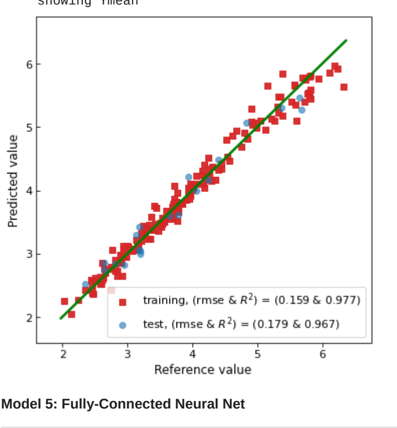


Model 4: Gaussian Process Regression

In [6]:

```
from matsml.models import GPR

# Model parameters
nfold_cv = 5
model_file = 'model_gpr.pkl'
verbosity = 0
n_restarts_optimizer = 100

model_params = {'nfold_cv': nfold_cv, 'n_restarts_optimizer': n_restarts_optimizer,
                'model_file': model_file, 'verbosity': verbosity}

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                      RBF
    nfold_cv                    5
    optimizer                   fmin_l_bfgs_b
    n_restarts_optimizer        100
    noise_lb                    0.1
    noise_ub                    10
    rmse_cv                     False
  Read data
    data file                   fp_hoips_S1_1dest.csv.gz
    data size                   192
    training size               89.6  %
    test size                   10.4  %
    x dimensionality            32
    y dimensionality            1
    y label(s)                  ['Ymean']
  Scaling x                     minmax
    xscaler saved in            xscaler.pkl
  Scaling y                     normalize
  Prepare train/test sets       random
  Training model w/ cross validation
    cv,rmse_train,rmse_test,rmse_opt: 0 0.158235 0.155520 0.155520
    cv,rmse_train,rmse_test,rmse_opt: 1 0.159902 0.155334 0.155334
    cv,rmse_train,rmse_test,rmse_opt: 2 0.149463 0.171093 0.155334
    cv,rmse_train,rmse_test,rmse_opt: 3 0.144789 0.261385 0.155334
    cv,rmse_train,rmse_test,rmse_opt: 4 0.157094 0.208261 0.155334
  GPR model trained, now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.159182
    unscaling y: normalize
       rmse test         Ymean            0.17919
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.159 & 0.977 )
    test, (rmse & R2) = ( 0.179 & 0.967 )
    showing Ymean
```



Model 5: Fully-Connected Neural Net

In [7]:

```
from matsml.models import FCNN

# model parameters
layers = [5,5]
epochs = 300
nfold_cv = 5
use_bias = True
model_file = 'model_fcnn.pkl'
loss = 'mse'
verbosity = 0
batch_size = 32
activ_funct = 'elu'
optimizer = 'nadam'

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}

model = FCNN(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                   fully connected NeuralNet w/ TensorFlow
    layers                      [5, 5]
    activ_funct                 elu
    epochs                      300
    optimizer                   nadam
    nfold_cv                    5
  Read data
    data file                   fp_hoips_S1_1dest.csv.gz
    data size                   192
    training size               89.6  %
    test size                   10.4  %
    x dimensionality            32
    y dimensionality            1
    y label(s)                  ['Ymean']
  Scaling x                     minmax
    xscaler saved in            xscaler.pkl
  Scaling y                     normalize
  Prepare train/test sets       random
  Building model                FCNN
  Training model w/ cross validation
    cv,rmse_train,rmse_test,rmse_opt: 0 0.184934 0.171607 0.171607
    cv,rmse_train,rmse_test,rmse_opt: 1 0.122511 0.225041 0.171607
    cv,rmse_train,rmse_test,rmse_opt: 2 0.127604 0.136820 0.136820
    cv,rmse_train,rmse_test,rmse_opt: 3 0.117731 0.148920 0.136820
    cv,rmse_train,rmse_test,rmse_opt: 4 0.104213 0.160592 0.136820
    Optimal ncv:  2 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.134738
    unscaling y: normalize
       rmse test         Ymean            0.148404
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.135 & 0.983 )
    test, (rmse & R2) = ( 0.148 & 0.977 )
    showing Ymean
```