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

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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. The raw data leading to this dataset is available at https://www.nature.com/articles/sdata201757.

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 fingeprint vector
fp_data = pd.read_csv('fp_hoips_S1_1dest.csv.gz')
print (fp_data.shape)
print (fp_data.columns)
```

```
  matsML, version 1.0.0
  *****
  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='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}
```

Model 1: Support Vector Regression

In [3]:

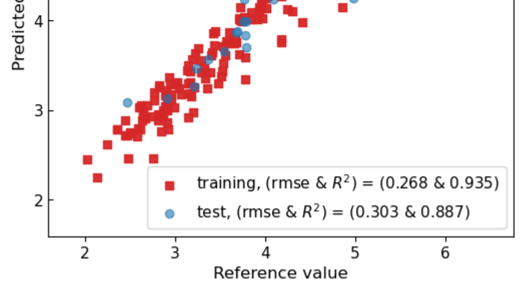
```
from matsml.models import SVecR

# 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)
```

```
  Learning fingerprinted/featured data
    algorithm                     support vector regression w/ scikit-learn
    kernel                        rbf
    regular_param                 2
    max_iter                      -1
    nfold_cv                      5
  Checking parameters
    all passed                    True
  Read data
    data file                     fp_hoips_S1_1dest.csv.gz
    data size                     192
    training size                 172 (89.6 %)
    test size                     20 (10.4 %)
    x dimensionality              32
    y dimensionality              1
    y label(s)                    ['Ymean']
  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 0.061336 0.065900 0.065900
    cv,rmse_train,rmse_test,rmse_opt: 1 0.059255 0.082091 0.065900
    cv,rmse_train,rmse_test,rmse_opt: 2 0.063549 0.065957 0.065900
    cv,rmse_train,rmse_test,rmse_opt: 3 0.061429 0.068594 0.065900
    cv,rmse_train,rmse_test,rmse_opt: 4 0.067078 0.074924 0.065900
  RFR model trained and saved in "model_svr.pkl"
  Now make predictions & invert scaling
    unscaling y: minmax
       rmse training     Ymean             0.267968
    unscaling y: minmax
       rmse test         Ymean             0.303103
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.268 & 0.935)
    test, (rmse & R2) = (0.303 & 0.887)
    showing Ymean
```



Model 2: Random Forest Regression

In [4]:

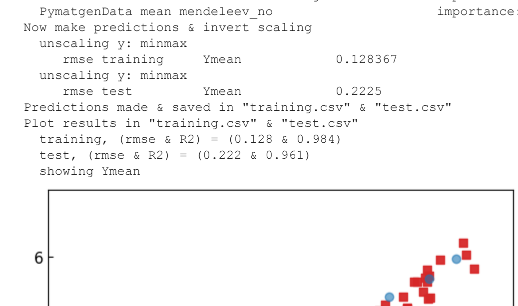
```
from matsml.models import RFR

# 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)
```

```
  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
  Checking parameters
    all passed                    True
  Read data
    data file                     fp_hoips_S1_1dest.csv.gz
    data size                     192
    training size                 172 (89.6 %)
    test size                     20 (10.4 %)
    x dimensionality              32
    y dimensionality              1
    y label(s)                    ['Ymean']
  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 0.019985 0.056001 0.056001
    cv,rmse_train,rmse_test,rmse_opt: 1 0.022022 0.049774 0.049774
    cv,rmse_train,rmse_test,rmse_opt: 2 0.020180 0.052332 0.049774
    cv,rmse_train,rmse_test,rmse_opt: 3 0.022245 0.055417 0.049774
    cv,rmse_train,rmse_test,rmse_opt: 4 0.020226 0.056037 0.049774
  RFR model trained and saved in "model_rfr.pkl"
  Top 10 features by importance
    MagpieData avg_dev GSvolume_pa                       importance: 0.457
    MatscholarElementData mean embedding 54              importance: 0.18
    MatscholarElementData std_dev embedding 116          importance: 0.127
    MatscholarElementData std_dev embedding 155          importance: 0.074
    MatscholarElementData mean embedding 4               importance: 0.044
    MatscholarElementData std_dev embedding 136          importance: 0.04
    MatscholarElementData mean embedding 140             importance: 0.028
    MatscholarElementData std_dev embedding 153          importance: 0.018
    MatscholarElementData mean embedding 170             importance: 0.016
    PymatgenData mean mendeleev_no                       importance: 0.004
  Now make predictions & invert scaling
    unscaling y: minmax
       rmse training     Ymean             0.128367
    unscaling y: minmax
       rmse test         Ymean             0.2225
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.128 & 0.984)
    test, (rmse & R2) = (0.222 & 0.961)
    showing Ymean
```



Model 3: Kernel Ridge Regression (KRR)

In [5]:

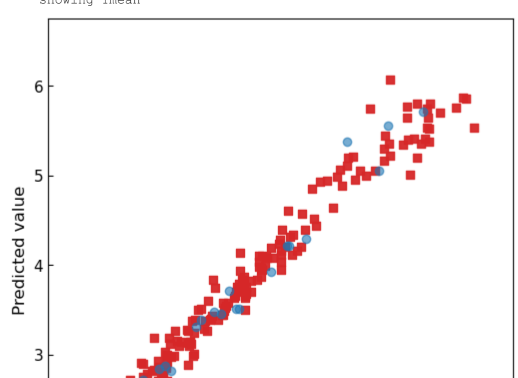
```
from matsml.models import KRR

# 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)
```

```
  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
  Checking parameters
    all passed                    True
  Read data
    data file                     fp_hoips_S1_1dest.csv.gz
    data size                     192
    training size                 172 (89.6 %)
    test size                     20 (10.4 %)
    x dimensionality              32
    y dimensionality              1
    y label(s)                    ['Ymean']
  Scaling x                       minmax
    xscaler saved in              xscaler.pkl
  Scaling y                       minmax
  Prepare train/test sets         random
  Building model                  KRR
  Training model w/ cross validation
  KRR model trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     Ymean             0.200223
    unscaling y: minmax
       rmse test         Ymean             0.154706
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.200 & 0.964)
    test, (rmse & R2) = (0.155 & 0.973)
    showing Ymean
```



Model 4: Gaussian Process Regression

In [6]:

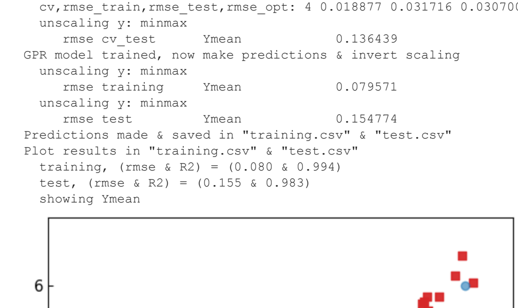
```
from matsml.models import GPR

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

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

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

```
  Learning fingerprinted/featured data
    algorithm                     gaussian process regression w/ scikit-learn
    nfold_cv                      5
    optimizer                     fmin_l_bfgs_b
    n_restarts_optimizer          100
    rmse_cv                       True
  Checking parameters
    all passed                    True
  Read data
    data file                     fp_hoips_S1_1dest.csv.gz
    data size                     192
    training size                 172 (89.6 %)
    test size                     20 (10.4 %)
    x dimensionality              32
    y dimensionality              1
    y label(s)                    ['Ymean']
  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 0.017592 0.036452 0.036452
    unscaling y: minmax
       rmse cv_test      Ymean             0.156809
    cv,rmse_train,rmse_test,rmse_opt: 1 0.018102 0.030700 0.030700
    unscaling y: minmax
       rmse cv_test      Ymean             0.132068
    cv,rmse_train,rmse_test,rmse_opt: 2 0.015147 0.032244 0.030700
    unscaling y: minmax
       rmse cv_test      Ymean             0.138708
    cv,rmse_train,rmse_test,rmse_opt: 3 0.018131 0.049642 0.030700
    unscaling y: minmax
       rmse cv_test      Ymean             0.213553
    cv,rmse_train,rmse_test,rmse_opt: 4 0.018877 0.031716 0.030700
    unscaling y: minmax
       rmse cv_test      Ymean             0.136439
  GPR model trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     Ymean             0.079571
    unscaling y: minmax
       rmse test         Ymean             0.154774
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.080 & 0.994)
    test, (rmse & R2) = (0.155 & 0.983)
    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)
```

```
  Learning fingerprinted/featured data
    algorithm                     fully connected NeuralNet w/ TensorFlow
    layers                        [5, 5]
    activ_funct                   elu
    epochs                        300
    optimizer                     nadam
    nfold_cv                      5
  Checking parameters
    all passed                    True
  Read data
    data file                     fp_hoips_S1_1dest.csv.gz
    data size                     192
    training size                 172 (89.6 %)
    test size                     20 (10.4 %)
    x dimensionality              32
    y dimensionality              1
    y label(s)                    ['Ymean']
  Scaling x                       minmax
    xscaler saved in              xscaler.pkl
  Scaling y                       minmax
  Prepare train/test sets         random
  Building model                  FCNN
  Training model w/ cross validation
    cv,rmse_train,rmse_test,rmse_opt: 0 0.053168 0.066369 0.066369
    cv,rmse_train,rmse_test,rmse_opt: 1 0.037757 0.042781 0.042781
    cv,rmse_train,rmse_test,rmse_opt: 2 0.031396 0.043164 0.042781
    cv,rmse_train,rmse_test,rmse_opt: 3 0.029349 0.040847 0.040847
    cv,rmse_train,rmse_test,rmse_opt: 4 0.028165 0.042264 0.040847
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     Ymean             0.137451
    unscaling y: minmax
       rmse test         Ymean             0.130711
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.137 & 0.983)
    test, (rmse & R2) = (0.131 & 0.979)
    showing Ymean
```