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. 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]:

```python
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]:

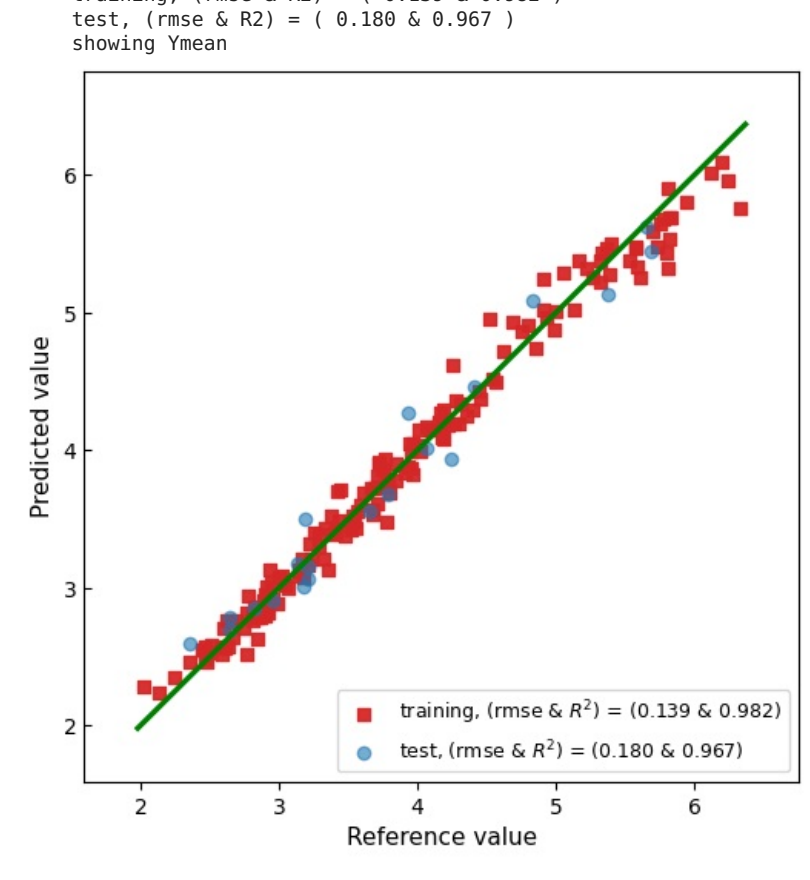
```python
# data parameters
data_file = 'fp_hoips_S1_1dest.csv.gz'
id_col = ['ID']
y_cols = ['Ymean']
comment_cols = []
n_trains = 0.9

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]:

```python
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 0.109104 0.235800 0.235800
    cv,rmse_train,rmse_test,rmse_opt: 1 0.122489 0.180884 0.180884
    cv,rmse_train,rmse_test,rmse_opt: 2 0.125387 0.172246 0.172246
    cv,rmse_train,rmse_test,rmse_opt: 3 0.124511 0.164694 0.164694
    cv,rmse_train,rmse_test,rmse_opt: 4 0.123357 0.262104 0.164694

  SVecR model trained and saved in "model_svr.pkl"

  Now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.138838
    unscaling y: normalize
       rmse test         Ymean            0.180482

  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) = ( 0.180 & 0.967 )
    showing Ymean
```

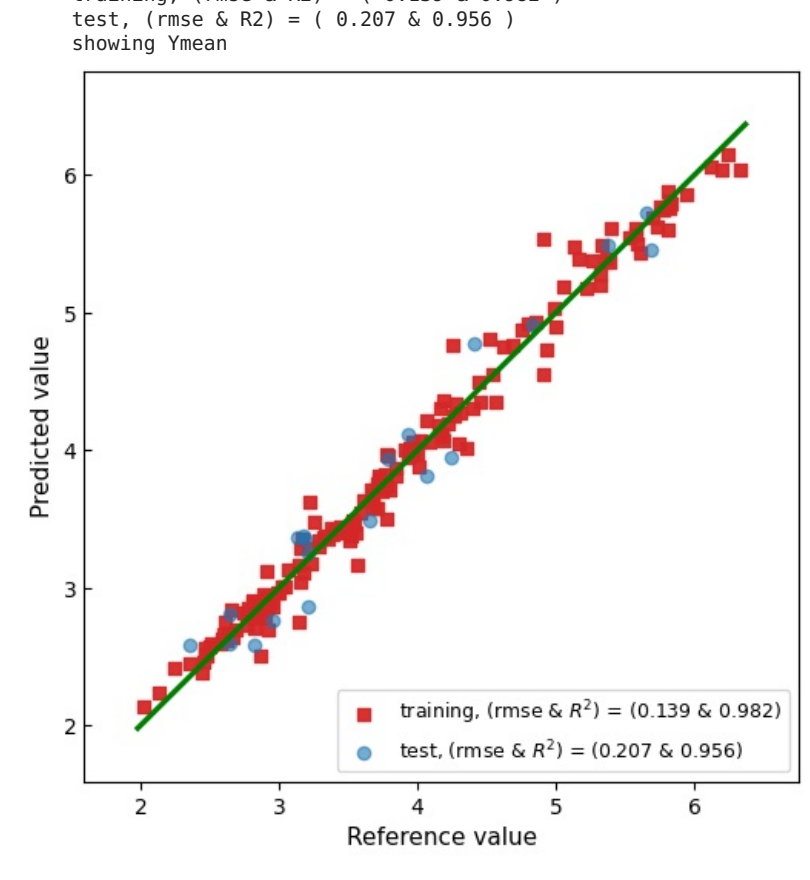


Model 2: Random Forest Regression

In [4]:

```python
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 = 'friedman_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                     friedman_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 0.087833 0.239798 0.239798
    cv,rmse_train,rmse_test,rmse_opt: 1 0.145265 0.071424 0.071424
    cv,rmse_train,rmse_test,rmse_opt: 2 0.141709 0.093664 0.071424
    cv,rmse_train,rmse_test,rmse_opt: 3 0.140723 0.099515 0.071424
    cv,rmse_train,rmse_test,rmse_opt: 4 0.143106 0.084604 0.071424

  RFR model trained and saved in "model_rfr.pkl"

  Top 10 features by importance
    MagpieData avg_dev GSvolume_pa                      importance: 0.58
    MatscholarElementData std_dev embedding 116         importance: 0.123
    MatscholarElementData std_dev embedding 136         importance: 0.08
    MatscholarElementData mean embedding 54             importance: 0.054
    MatscholarElementData std_dev embedding 155         importance: 0.051
    MatscholarElementData mean embedding 4              importance: 0.044
    MatscholarElementData mean embedding 170            importance: 0.027
    MatscholarElementData std_dev embedding 153         importance: 0.016
    MatscholarElementData mean embedding 140            importance: 0.009
    PymatgenData mean mendeleev_no                      importance: 0.007

  Now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.139016
    unscaling y: normalize
       rmse test         Ymean            0.207248

  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) = ( 0.207 & 0.956 )
    showing Ymean
```

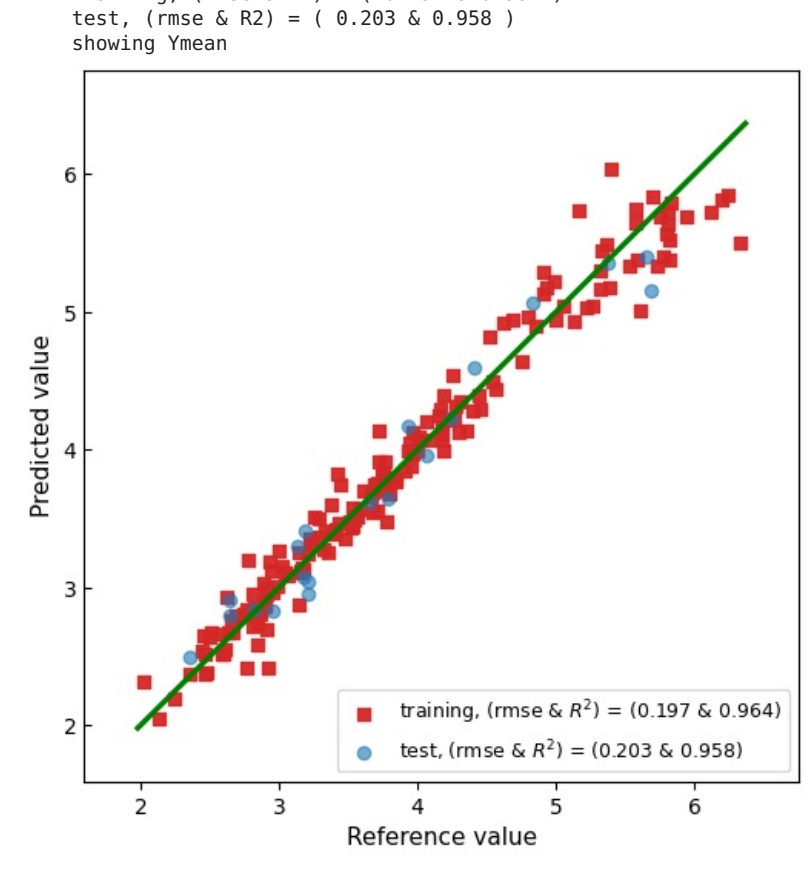


Model 3: Kernel Ridge Regression (KRR)

In [5]:

```python
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            0.197194
    unscaling y: normalize
       rmse test         Ymean            0.202596

  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
```

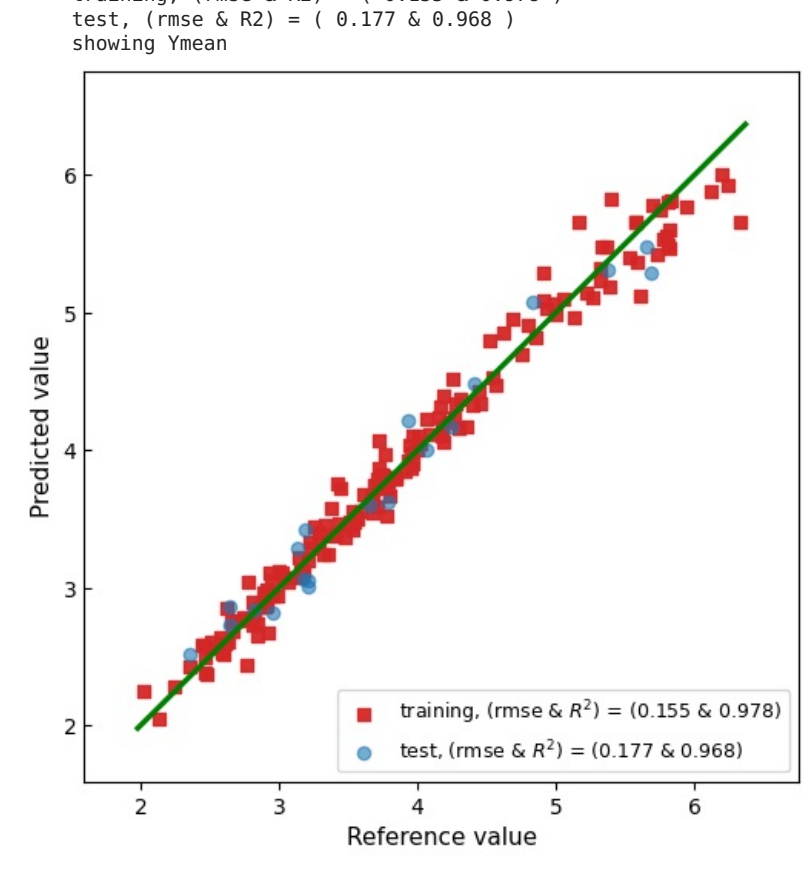


Model 4: Gaussian Process Regression

In [6]:

```python
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 0.155248 0.162883 0.162883
    cv,rmse_train,rmse_test,rmse_opt: 1 0.156474 0.215593 0.162883
    cv,rmse_train,rmse_test,rmse_opt: 2 0.156251 0.220876 0.162883
    cv,rmse_train,rmse_test,rmse_opt: 3 0.150226 0.204543 0.162883
    cv,rmse_train,rmse_test,rmse_opt: 4 0.155482 0.167650 0.162883

  GPR model trained, now make predictions & invert scaling
    unscaling y: normalize
       rmse training     Ymean            0.155389
    unscaling y: normalize
       rmse test         Ymean            0.176896

  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.155 & 0.978 )
    test, (rmse & R2) = ( 0.177 & 0.968 )
    showing Ymean
```



Model 5: Fully-Connected Neural Net

In [7]:

```python
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)
```

```
2025-12-06 22:16:06.325098: I tensorflow/core/platform/cpu_feature_guard.cc:210] This TensorFlow binary is optimized to use available CPU instructions in performance-critical operations.
To enable the following instructions: AVX2 AVX_VNNI FMA, in other operations, rebuild TensorFlow with the appropriate compiler flags.
```

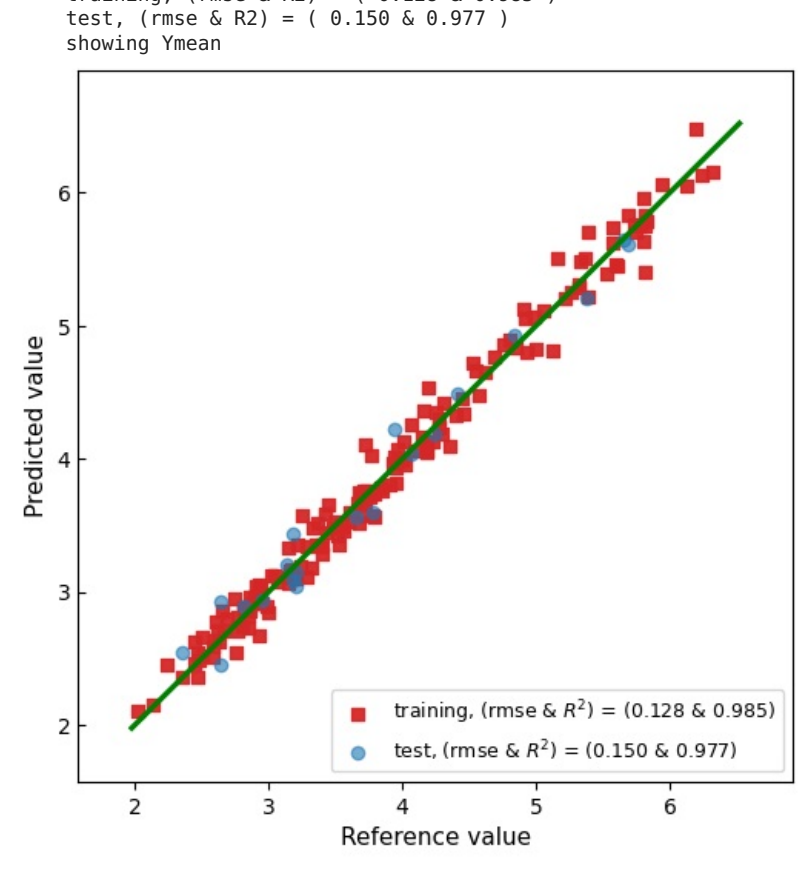
```
  Checking parameters
    model_file not ends with ".weights.h5", renamed

  Learning fingerprinted/featured data
    algorithm                     fully connected NeuralNet w/ TensorFlow
    layers                        [5, 5]
    activ_funct                   elu
    epochs                        300
    optimizer                     nadam
    nfold_cv                      5
    verbosity                     0

  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
```

```
WARNING: All log messages before absl::InitializeLog() is called are written to STDERR
I0000 00:00:1765077367.510046 1027169 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 capability: 7.5
```

```
  Training model w/ cross validation
```

```
2025-12-06 22:16:08.108660: I external/local_xla/xla/service/service.cc:163] XLA service 0x152efcd5a5c0 initialized for platform CUDA (this does not guarantee that XLA will be used). Devices:
2025-12-06 22:16:08.108672: I external/local_xla/xla/service/service.cc:171]   StreamExecutor device (0): NVIDIA GeForce RTX 2060, Compute Capability 7.5
2025-12-06 22:16:08.115108: I tensorflow/compiler/mlir/tensorflow/utils/dump_mlir_util.cc:269] disabling MLIR crash reproducer, set env var `MLIR_CRASH_REPRODUCER_DIRECTORY` to enable.
2025-12-06 22:16:08.124861: I external/local_xla/xla/stream_executor/cuda/cuda_dnn.cc:473] Loaded cuDNN version 90501
I0000 00:00:1765077368.171835 1027267 device_compiler.h:196] Compiled cluster using XLA!  This line is logged at most once for the lifetime of the process.
```

```
5/5 [==============================] - 0s 581us/step
2/2 [==============================] - 0s 797us/step
    cv,rmse_train,rmse_test,rmse_opt: 0 0.197491 0.241717 0.241717
5/5 [==============================] - 0s 585us/step
2/2 [==============================] - 0s 698us/step
    cv,rmse_train,rmse_test,rmse_opt: 1 0.137095 0.219245 0.219245
5/5 [==============================] - 0s 496us/step
2/2 [==============================] - 0s 802us/step
    cv,rmse_train,rmse_test,rmse_opt: 2 0.119732 0.191045 0.191045
5/5 [==============================] - 0s 527us/step
2/2 [==============================] - 0s 738us/step
    cv,rmse_train,rmse_test,rmse_opt: 3 0.119843 0.134300 0.134300
5/5 [==============================] - 0s 573us/step
2/2 [==============================] - 0s 896us/step
    cv,rmse_train,rmse_test,rmse_opt: 4 0.110045 0.155503 0.134300
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
6/6 [==============================] - 0s 557us/step
    unscaling y: normalize
       rmse training     Ymean            0.127827
1/1 [==============================] - 0s 11ms/step
    unscaling y: normalize
       rmse test         Ymean            0.149506
  Predictions made & saved in "training.csv" & "test.csv"

  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = ( 0.128 & 0.985 )
    test, (rmse & R2) = ( 0.150 & 0.977 )
    showing Ymean
```



In [ ]: