ComparePolynom

October 11, 2019

1 Compare polynomial fitting with neural network regressor

1.1 In this example, a noisy cosine function is fitted by 3 polynomes of different orders, and 3 neural networks with different layers sizes.

1.1.1 Import usefull libraries.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

1.1.2 The polynomial fit is performed using the scikit modules.

[2]:
```
# Import stuff to perform the polynomial fit
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
# Import tool to compute rms
from sklearn.metrics import mean_squared_error
# Import the TMNI. If not installed, install it
try:
    import mwinai
except:
    !pip install -U git+https://github.com/
 ↪taller-mexicano-de-nebulosas-ionizadas/AI.git
    import mwinai
```

```
/home/morisset/anaconda3/lib/python3.7/site-
packages/sklearn/externals/joblib/__init__.py:15: DeprecationWarning:
sklearn.externals.joblib is deprecated in 0.21 and will be removed in 0.23.
Please import this functionality directly from joblib, which can be installed
with: pip install joblib. If this warning is raised when loading pickled models,
you may need to re-serialize those models with scikit-learn 0.21+.
  warnings.warn(msg, category=DeprecationWarning)
Using TensorFlow backend.
```

1.1.3 Define the function we want to interpolate.

[3]:
```
def true_fun(x):
    return np.cos(1.5 * np.pi * x)
```

1.1.4 Define some parameters. The X_train and y_train sets are used to determine the polynome coefficients and also to train the neural networks.

[4]:
```
# A random seed to reproduce the results
np.random.seed(0)

# The number of points used to fit the function
n_samples = 30

# Noise to be added to the points used to fit the function
noise = 0.1

# The training set: n_samples X points, with the noisy correspoing y
X = np.sort(np.random.rand(n_samples))
y = true_fun(X) + np.random.randn(n_samples) * noise
X_train = X
y_train_true = y

# The set of points to verify the fit quality
X_test = np.linspace(0, 1, 100)
y_test_true = true_fun(X_test)
```

1.1.5 The pipeline object is defined to fit the X_train - y_train data sets. The order of the polynome is set to 2.

[5]:
```
degree = 2
polynomial_features = PolynomialFeatures(degree=degree,
                                         include_bias=False)
linear_regression = LinearRegression()
pipeline = Pipeline([("polynomial_features", polynomial_features),
                     ("linear_regression", linear_regression)])
pipeline.fit(X_train[:, np.newaxis], y_train_true);
```

1.1.6 The RMS of the fit computed on the dataused to determine the coefficients is computed.

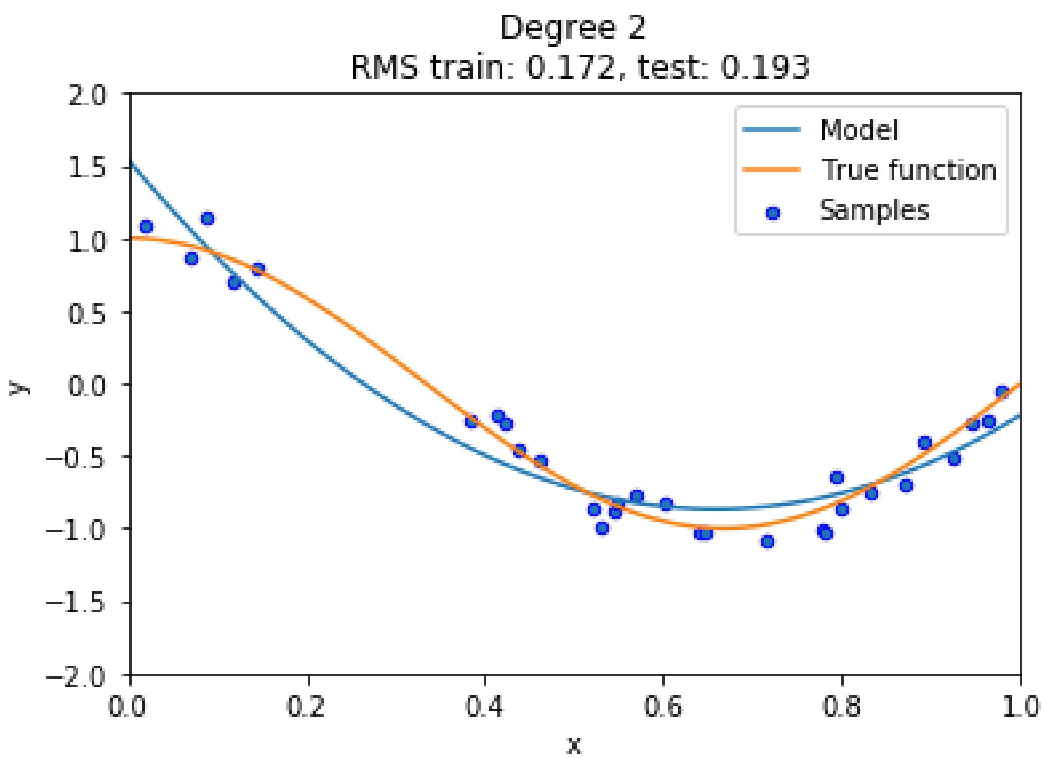
[6]:
```
y_train = pipeline.predict(X_train[:, np.newaxis])
rms_train = np.sqrt(mean_squared_error(y_train,y_train_true))
```

1.1.7 The RMS of the fit computed on the test sample (100 points between 0 and 1) is computed.

[7]:
```
y_test = pipeline.predict(X_test[:, np.newaxis])
rms_test = np.sqrt(mean_squared_error(y_test,y_test_true))
```

A plot is done to show the original function, the training sample and the polynomial fit.

[8]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, y_test_true, label="True function")
ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_xlim((0, 1))
ax.set_ylim((-2, 2))
ax.legend(loc="best")
ax.set_title("Degree {}\n RMS train: {:.3f}, test: {:.3f}".format(degree,
             rms_train, rms_test));
```



1.1.8 A Neural Network is used on the same data points.

1.1.9 It is trained on the training sets. Hyper-parameters can be changed.

[23]:
```
RM = mwinai.manage_RM(RM_type='SK_ANN', X_train=X_train, y_train=y_train_true,␣
 ↪scaling=True,
                  verbose=True, random_seed=10)
RM.init_RM(hidden_layer_sizes=(2,),
           tol=1e-6, max_iter=10000,
           activation='tanh',
           solver='adam')
RM.train_RM()
```

```
Instantiation. V 0.17
Training set size = 30, Test set size = 0
Train data scaled.
Test data scaled.
Training set size = 30, Test set size = 0
Training set size = 30, Test set size = 0
Regression Model SK_ANN
Training 1 inputs for 1 outputs with 30 data
RM trained, with 4280 iterations. Score = 0.970
MLPRegressor(activation='tanh', alpha=0.0001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(2,), learning_rate='constant',
             learning_rate_init=0.001, max_iter=10000, momentum=0.9,
             n_iter_no_change=10, nesterovs_momentum=True, power_t=0.5,
             random_state=10, shuffle=True, solver='adam', tol=1e-06,
             validation_fraction=0.1, verbose=False, warm_start=False)
Training time 1.0 s.
```

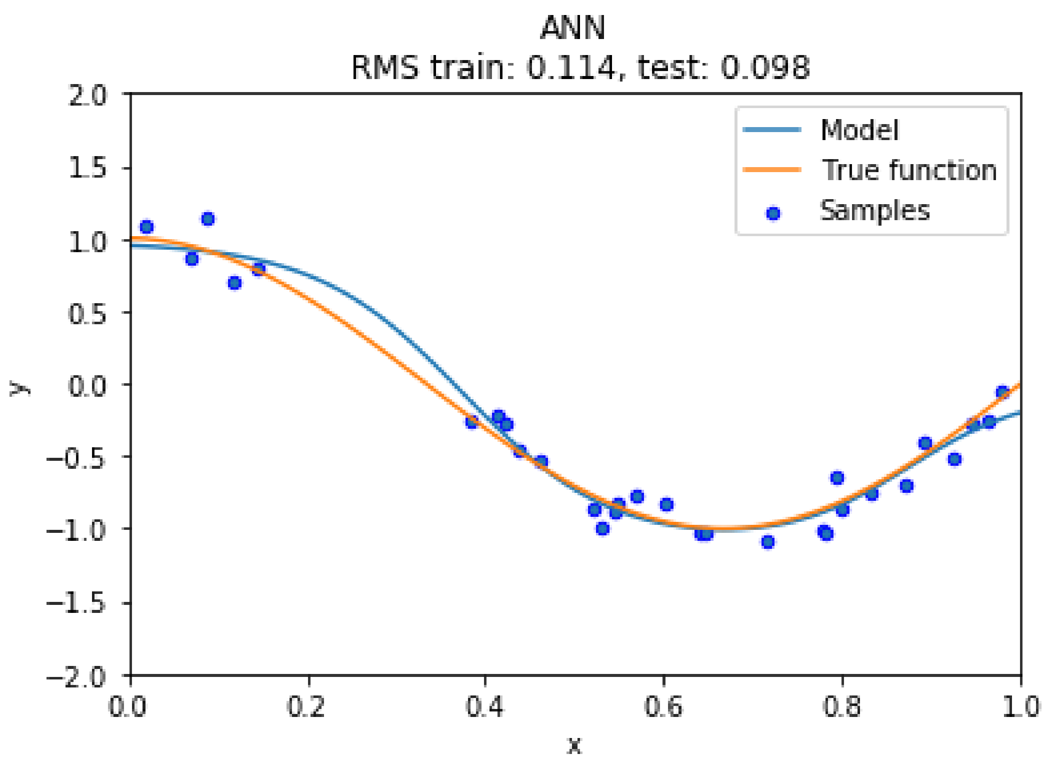
1.1.10 Predictions of the ANN are performed on the training and test sets.

[24]:
```
RM.set_test(X_train)
RM.predict(scoring=False)
y_train = RM.pred
rms_train = np.sqrt(mean_squared_error(y_train, y_train_true))
RM.set_test(X_test)
RM.predict(scoring=False)
y_test = RM.pred
rms_test = np.sqrt(mean_squared_error(y_test, y_test_true))
```

```
Test data scaled.
Training set size = 30, Test set size = 30
Predicting from 1 inputs to 1 outputs using 30 data in 0.00 secs.
Test data scaled.
Training set size = 30, Test set size = 100
Predicting from 1 inputs to 1 outputs using 100 data in 0.00 secs.
```

1.1.11 A plot is done to show the original function, the training sample and the polynomial fit.

[25]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, y_test_true, label="True function")
ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_xlim((0, 1))
ax.set_ylim((-2, 2))
ax.legend(loc="best")
ax.set_title("ANN\n RMS train: {:.3f}, test: {:.3f}".format(
             rms_train, rms_test));
```

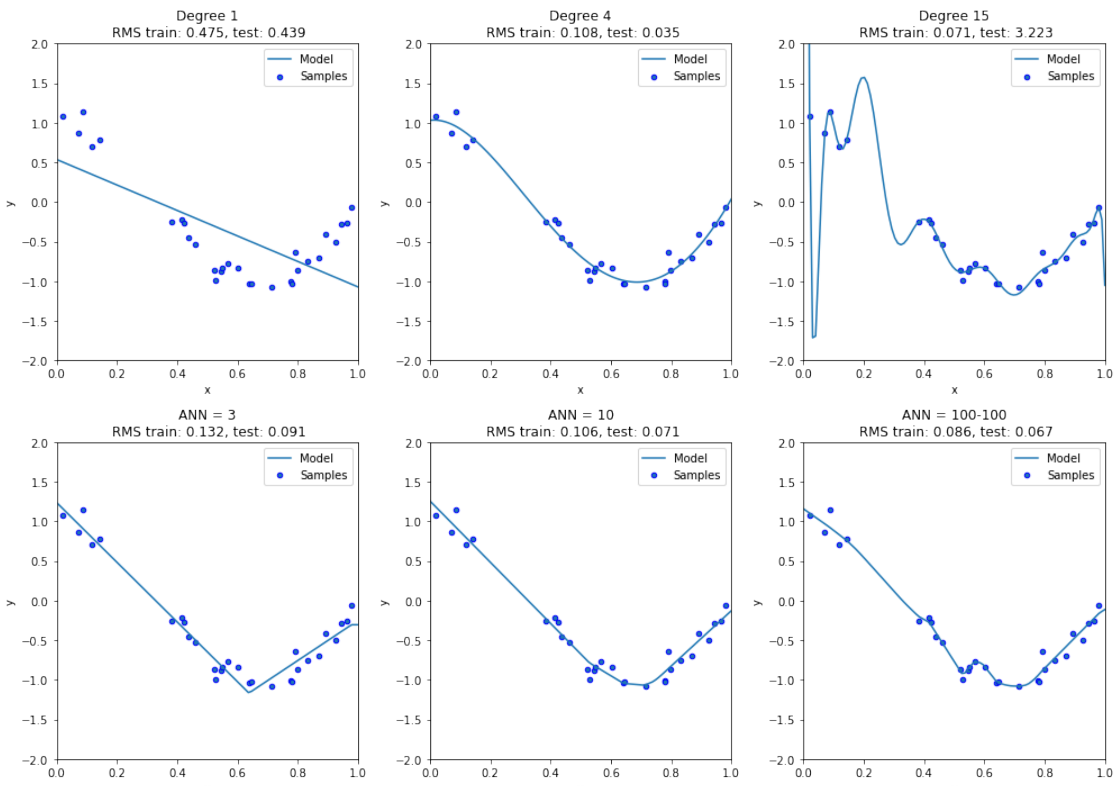


A comparison is made between 3 polynomial fits and 3 ANN computations.

[26]:
```
f, axes = plt.subplots(2, 3, figsize=(14, 10))

degrees = [1, 4, 15]
for i in range(len(degrees)):
    ax = axes[0,i]

    polynomial_features = PolynomialFeatures(degree=degrees[i],
```

```
                                                 include_bias=False)
    linear_regression = LinearRegression()
    pipeline = Pipeline([("polynomial_features", polynomial_features),
                         ("linear_regression", linear_regression)])
    pipeline.fit(X_train[:, np.newaxis], y_train_true)
    y_train = pipeline.predict(X_train[:, np.newaxis])
    y_test = pipeline.predict(X_test[:, np.newaxis])
    rms_train = np.sqrt(mean_squared_error(y_train,y_train_true))
    rms_test = np.sqrt(mean_squared_error(y_test,y_test_true))
    ax.plot(X_test, y_test, label="Model")
    #ax.plot(X_test, y_test_true, label="True function")
    ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
    ax.set_xlabel("x")
    ax.set_ylabel("y")
    ax.set_xlim((0, 1))
    ax.set_ylim((-2, 2))
    ax.legend(loc="best")
    ax.set_title("Degree {}\n RMS train: {:.3f}, test: {:.3f}".format(␣
 ↪degrees[i],
                 rms_train, rms_test))

hidden_layer_sizes_set = ( (3,), (10,), (100, 100))
hidden_layer_sizes_strs = ('3', '10', '100-100')
for i in range(len(hidden_layer_sizes_set)):
    scaleit=True
    RM = mwinai.manage_RM(RM_type='SK_ANN', X_train=X_train,␣
 ↪y_train=y_train_true, scaling=scaleit,
                      verbose=False, random_seed=10)
    RM.init_RM(hidden_layer_sizes=hidden_layer_sizes_set[i],
               tol=1e-6, max_iter=10000,
               activation='relu',
               solver='adam')
    RM.train_RM()
    RM.set_test(X_train)
    RM.predict(scoring=False)
    y_train = RM.pred
    RM.set_test(X_test)
    RM.predict(scoring=False)
    y_test = RM.pred
    rms_train = np.sqrt(mean_squared_error(y_train, y_train_true))
    rms_test = np.sqrt(mean_squared_error(y_test, y_test_true))
    ax = axes[1,i]
    ax.plot(X_test, y_test, label="Model")
    #ax.plot(X_test, y_test_true, label="True function")
    ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
    ax.set_xlabel("x")
    ax.set_ylabel("y")
```

```
    ax.set_xlim((0, 1))
    ax.set_ylim((-2, 2))
    ax.legend(loc="best")
    ax.set_title("ANN = {}\n RMS train: {:.3f}, test: {:.3f}".
 ↪format(hidden_layer_sizes_strs[i],
                    rms_train, rms_test))
f.tight_layout()
```



[ ]: