ComparePolynom

September 1, 2020

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
import pandas as pd
%matplotlib inline
```

1.2 Polynomial fit

1.2.1 The polynomial fit is performed using the scikit modules.

[2]:
```
import tensorflow
print(tensorflow.__version__)
```

```
2.0.0
```

[3]:
```
# Import stuff to perform the polynomial fit
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.pipeline import Pipeline
# Import tool to compute rms
from sklearn.metrics import mean_squared_error
# Import the TMNI. If not installed, install it
try:
    import ai4neb
except:
    !pip install -U git+https://github.com/morisset/AI4neb.git
    import ai4neb
```

1.2.2 Define the function we want to interpolate.

[4]:
```
def true_fun(x):
    return np.cos(1.5 * np.pi * x)
```

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

[5]:
```
# 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)
```

1.2.4 A fit to the data points is done using a polynome or order 3

[6]:
```
degree = 3
polynomial_features = PolynomialFeatures(degree=degree,
                                         include_bias=False)
model = LinearRegression()
X_TRANSF = polynomial_features.fit_transform(X_train[:, np.newaxis])
model.fit(X_TRANSF, y_train_true)
```

[6]:
```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None, normalize=False)
```

1.2.5 The RMS of the fit computed on the training set used to determine the coefficients is computed.

[7]:
```
y_train = model.predict(X_TRANSF)
rms_train = np.sqrt(mean_squared_error(y_train,y_train_true))
```

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

[8]:
```
y_test = model.predict(polynomial_features.fit_transform(X_test[:, np.newaxis]))
rms_test = np.sqrt(mean_squared_error(y_test,y_test_true))
```

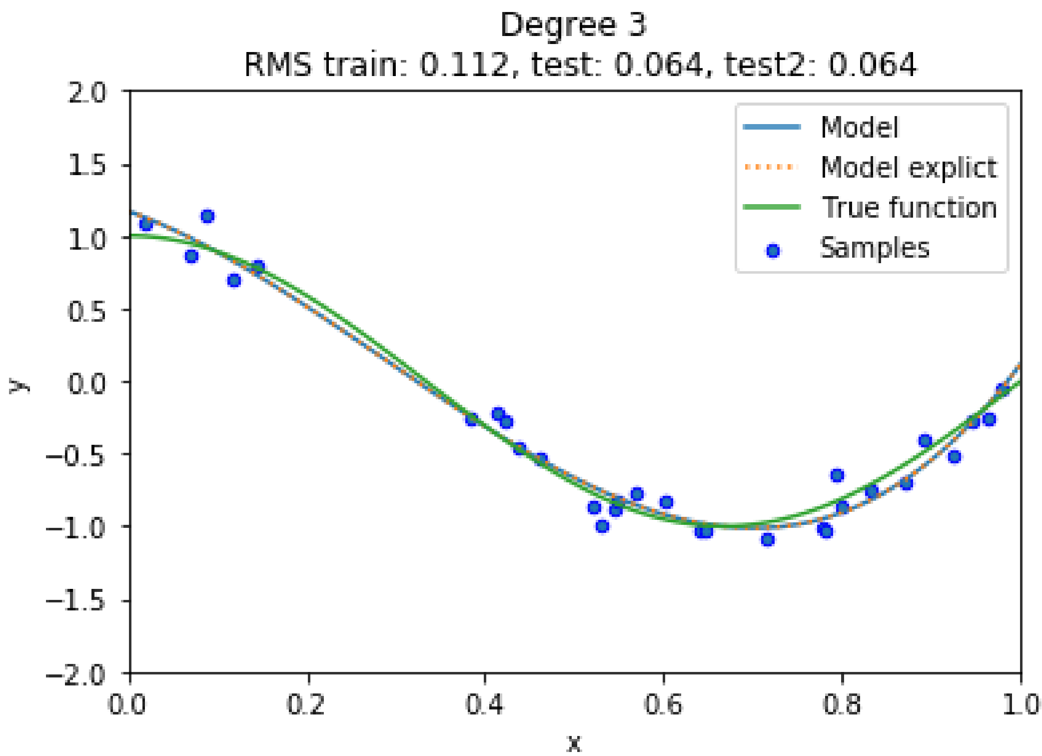
1.2.7 A lambda function of the fit is obtained using the determined coefficients:

$$y(X) = A + B.X + C.X^2 + D.X^3$$

[9]:
```
poly = lambda x: model.intercept_ + model.coef_[0] * x + model.coef_[1] * x**2␣
↪+ model.coef_[2] * x**3
```

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

[10]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, poly(X_test), label="Model explict", ls=':')
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}, test2: {:.3f}".
↪format(degree,
             rms_train, rms_test, rms_test));
```

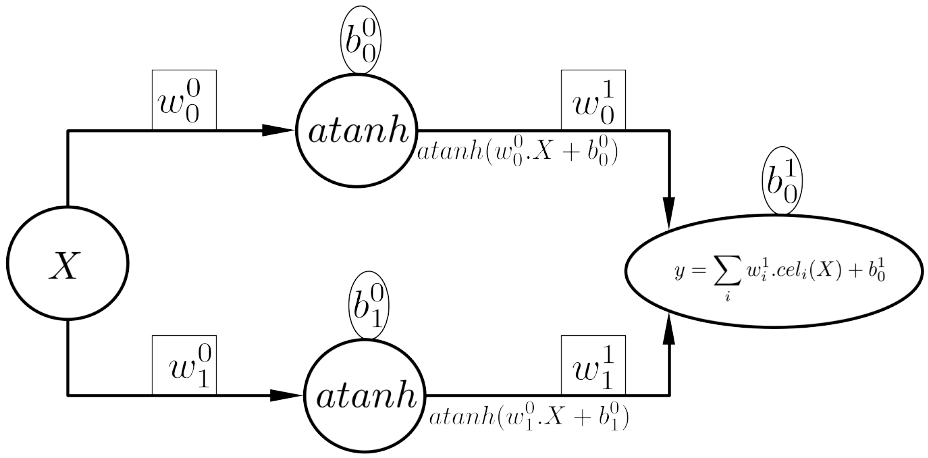


1.3 A Neural Network is used on the same data points.

1.3.1 General description of the ANN

[13]:
```
from IPython.display import Image
Image(filename = "ANN_1_2.png", width = 800)
```

[13]:



1.3.2 The neuron network can be explictly computed with the weigths and the biases, a total of 7 parameters.

1.3.3 Hidden layer:

$$cel_i(X) = atanh(w_i^0.X + b_i^0)$$

1.3.4 Output:

$$y(X) = \sum_i w_i^1.cel_i(X) + b_0^1 = w_0^1.atanh(w_0^0.X + b_0^0) + w_1^1.atanh(w_1^0.X + b_1^0) + b_0^1$$

1.3.5 The weights and biases of the individual neurons can be obtained.

- `coefs_ are the weigths of each synapse. It is a 3 dims list: coefs_[i_layer][i_previous_neuron][i_neuron]`
- `intercepts are the biases of each neuron: intercept_[i_layer][i_neuron]`

1.3.6 It is trained on the training sets. Hyper-parameters can be changed. The network is the minimal possible: 1 layer of 2 cells. Each cell is performing an *atanh* operation.

[11]:
```
RM = ai4neb.manage_RM(RM_type='SK_ANN', X_train=X_train, y_train=y_train_true,␣
↪scaling=False,
                     verbose=True, random_seed=10)
RM.init_RM(hidden_layer_sizes=(2,),
           tol=1e-7, max_iter=20000,
           activation='tanh',
```

```
            solver='adam')
RM.train_RM()
```

```
Instantiation. V 0.17
Training set size = 30, Test set size = 0
Training set size = 30, Test set size = 0
Regression Model SK_ANN
WARNING: training data not scaled
Training 1 inputs for 1 outputs with 30 data
RM trained, with 10633 iterations. Score = 0.974
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_fun=15000, max_iter=20000,
             momentum=0.9, n_iter_no_change=10, nesterovs_momentum=True,
             power_t=0.5, random_state=10, shuffle=True, solver='adam',
             tol=1e-07, validation_fraction=0.1, verbose=False,
             warm_start=False)
Training time 2.4 s.
```

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

[12]:
```
RM.set_test(X_train)
RM.predict()
y_train = RM.pred
rms_train = np.sqrt(mean_squared_error(y_train, y_train_true))
RM.set_test(X_test)
RM.predict()
y_test = RM.pred
rms_test = np.sqrt(mean_squared_error(y_test, y_test_true))
```

```
WARNING: test data not scaled
Predicting from 1 inputs to 1 outputs using 30 data in 0.00 secs.
WARNING: test data not scaled
Predicting from 1 inputs to 1 outputs using 100 data in 0.00 secs.
```

[14]:
```
rm = RM.RMs[0]
print(rm.coefs_)
print(rm.intercepts_)
```

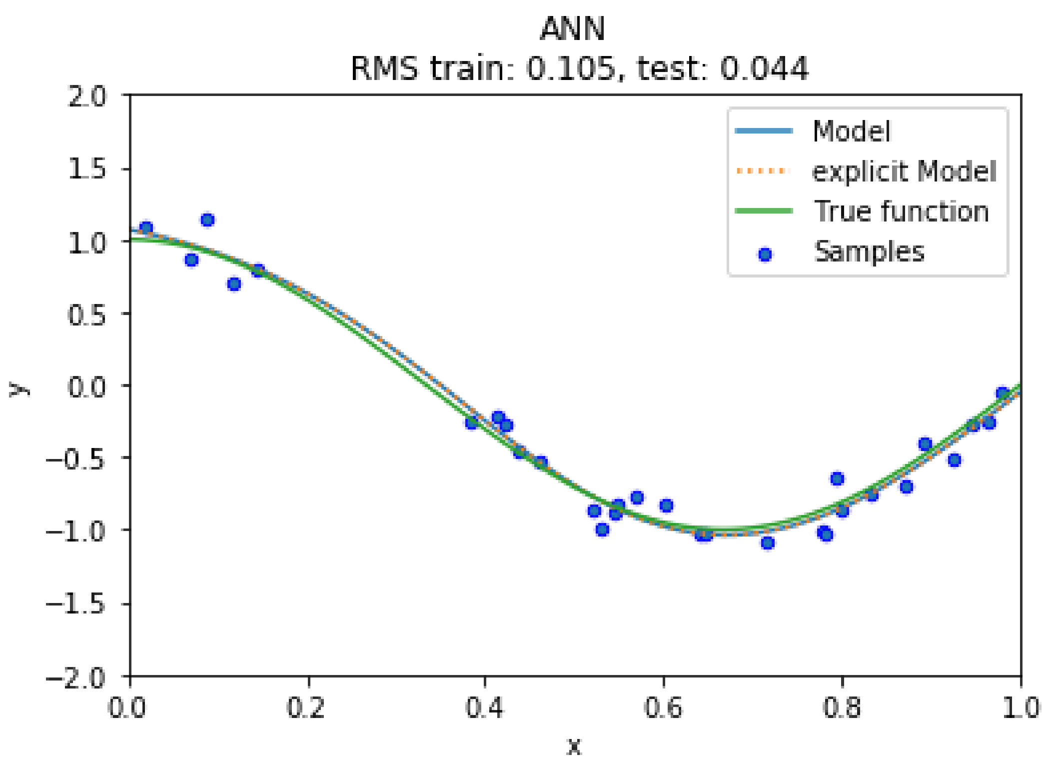
```
[array([[-3.27986762,  2.38700192]]), array([[1.85081241],
       [2.18101657]])]
[array([ 1.35423595, -2.3252666 ]), array([1.58891653])]
```

[15]:
```
activation = lambda x: np.tanh(x)
cel_0 = lambda x: activation(x * rm.coefs_[0][0][0] + rm.intercepts_[0][0])
cel_1 = lambda x: activation(x * rm.coefs_[0][0][1] + rm.intercepts_[0][1])
```

```
output = lambda x: cel_0(x) * rm.coefs_[1][0][0] + cel_1(x) * rm.
↪coefs_[1][1][0] + rm.intercepts_[1][0]
```

1.3.8 A plot is done to show the original function, the training sample, the ANN regression and the explicit ANN.

[16]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, output(X_test), label="explicit Model", ls=':')
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));
```



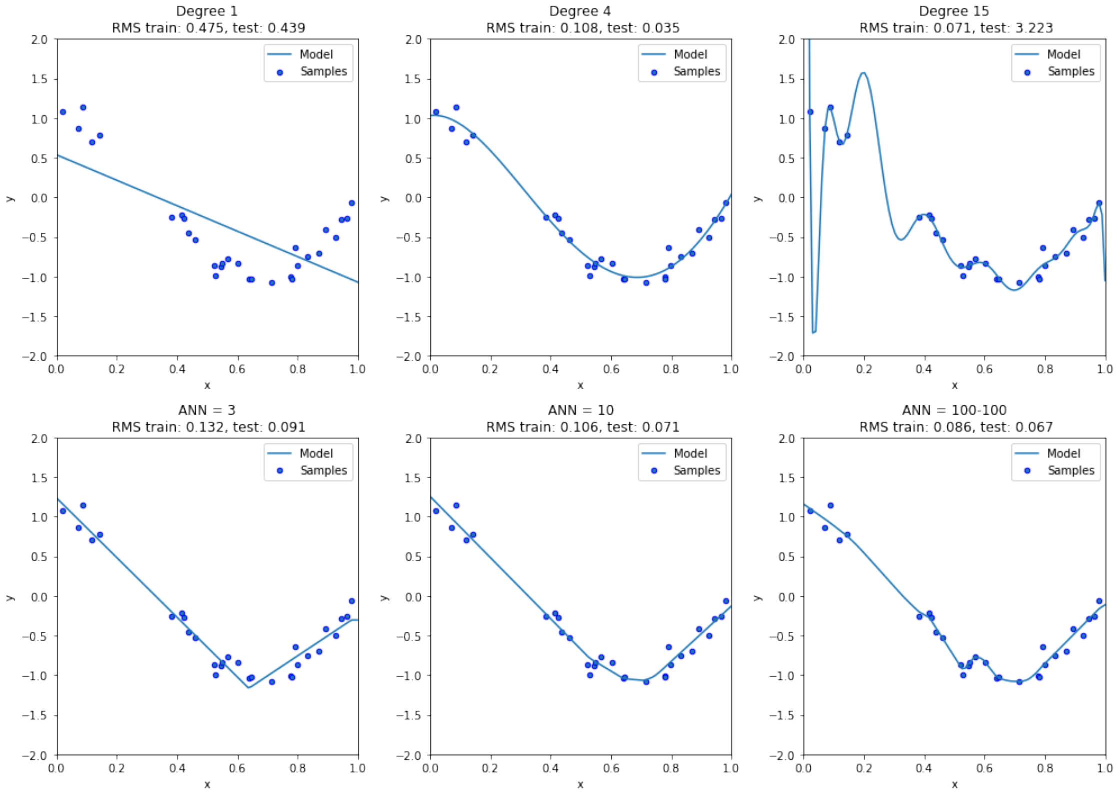
1.4 A comparison is made between 3 polynomial fits and 3 ANN computations (using RELU activation functions).

[17]:
```
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 = ai4neb.manage_RM(RM_type='SK_ANN', X_train=X_train,␣
 ↪y_train=y_train_true, scaling=scaleit,
                      verbose=True, random_seed=10)
    RM.init_RM(hidden_layer_sizes=hidden_layer_sizes_set[i],
               tol=1e-6, max_iter=10000,
#               epochs = 10000,
               activation='relu',
               solver='adam')
    RM.train_RM()
    RM.set_test(X_train)
    RM.predict()
    y_train = RM.pred
```

```
    RM.set_test(X_test)
    RM.predict()
    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()
```

```
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 5405 iterations. Score = 0.959
MLPRegressor(activation='relu', alpha=0.0001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(3,), learning_rate='constant',
             learning_rate_init=0.001, max_fun=15000, 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 1.5 s.
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.
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 2518 iterations. Score = 0.974
MLPRegressor(activation='relu', alpha=0.0001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(10,), learning_rate='constant',
             learning_rate_init=0.001, max_fun=15000, 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 0.7 s.
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.
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 893 iterations. Score = 0.983
MLPRegressor(activation='relu', alpha=0.0001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(100, 100), learning_rate='constant',
             learning_rate_init=0.001, max_fun=15000, 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 0.6 s.
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.
```


Degree 1
RMS train: 0.475, test: 0.439
Degree 4
RMS train: 0.108, test: 0.035
Degree 15
RMS train: 0.071, test: 3.223
ANN = 3
RMS train: 0.132, test: 0.091
ANN = 10
RMS train: 0.106, test: 0.071
ANN = 100-100
RMS train: 0.086, test: 0.067
Model
Samples
x
y