ComparePolynom

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1 Compare polynomial fitting with neural network regressor

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 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:

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

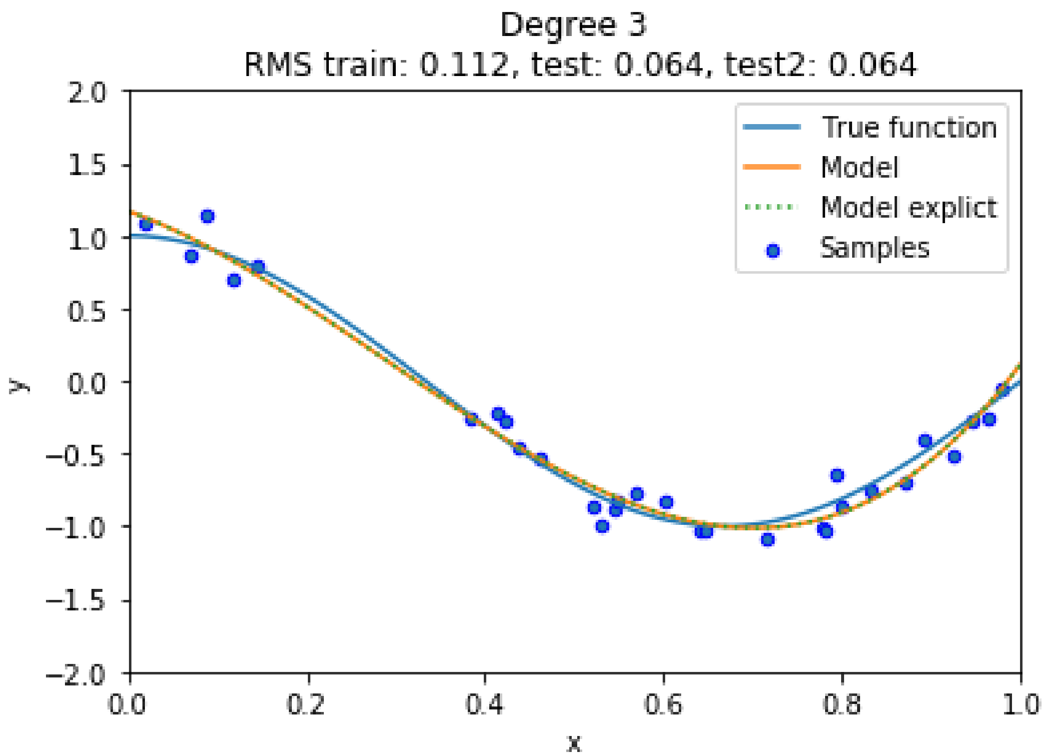
[9]:
```
print(model.intercept_, model.coef_)
```

```
1.169394115831641 [-2.19617614 -7.05669992  8.202858  ]
```

[10]:
```
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.

[11]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test_true, label="True function")
ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, poly(X_test), label="Model explict", ls=':')
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.

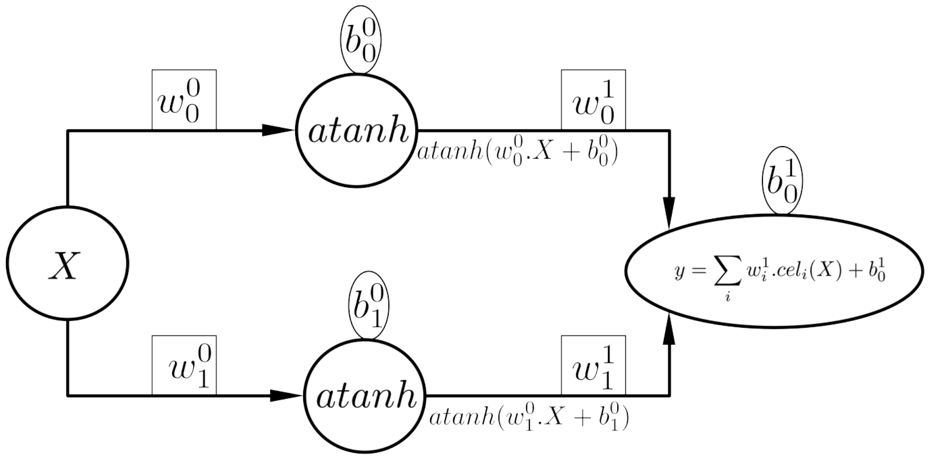
1.3.1 General description of the ANN

An Analogic Neural Network in "only" a linear combination of series of simple "activation" functions, which are very basic function going smoothly from one value for x < 0 to another value for x > 0, for example from -1 to 1 in the case of $atanh(x)$. The coefficients of the combination are called **weigths**, and the constant parameter is called **bias**.

In the following example, 2 neurons are considered. Each neuron apply the activation *atanh* function to a linear transformation of the previous layer, in this case the X input. The output of each neuron is sent to the next layer, here the final output y, which also linearly combine what comes from the hidden layer. Each connection between neurons (synapse) has a **weight** parameter, and each neuron has a **bias** parameter, to define these linear combinations.

[12]:
```
from IPython.display import Image
Image(filename = "ANN_1_2.png", width = 800)
```

[12]:



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

Hidden layer:

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

Output:

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

1.3.3 The weights and biases of the individual neurons can be obtained from the scikit object.

- `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]`

1.3.4 The ANN 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.

[13]:
```
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 2.3 s.
```

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

[14]:
```
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.
```

1.3.6 Parameters of the ANN from the scikit objects

[15]:
```
rm = RM.RMs[0]
print(rm.coefs_)
print(rm.intercepts_)
```

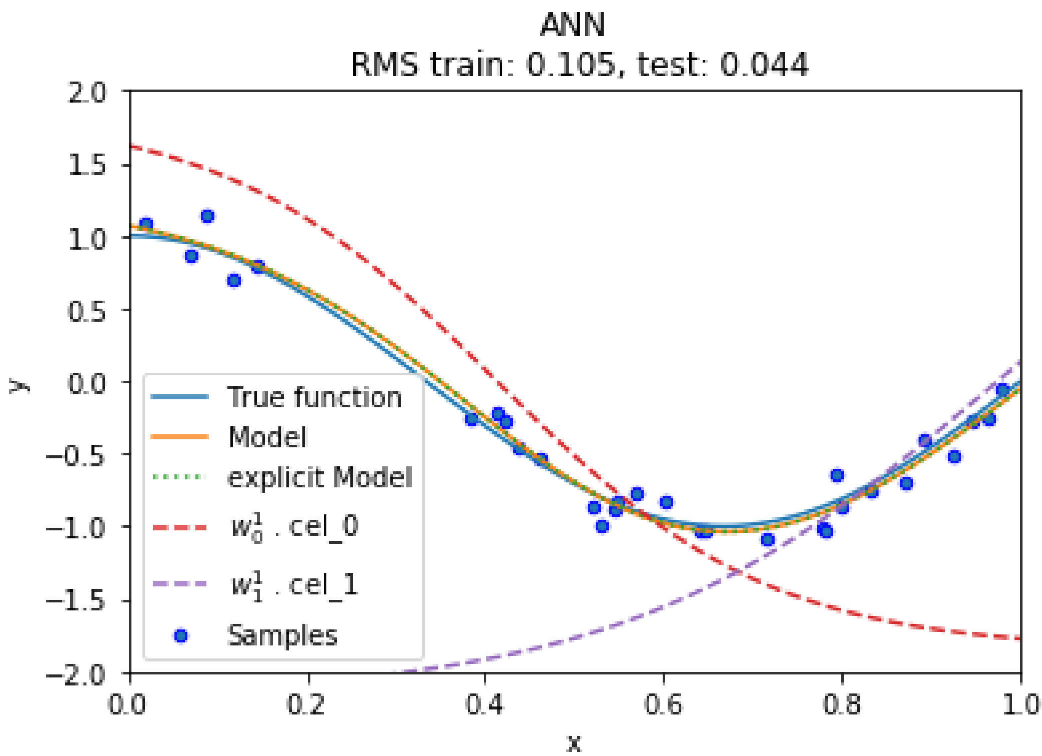
```
[array([[-3.27986762,  2.38700192]]), array([[1.85081241],
       [2.18101657]])]
[array([ 1.35423595, -2.3252666 ]), array([1.58891653])]
```

1.3.7 The explicit form of the ANN is computed

[16]:
```
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.

[17]:
```
f, ax = plt.subplots()
ax.plot(X_test, y_test_true, label="True function")
ax.scatter(X, y, edgecolor='b', s=20, label="Samples")
ax.plot(X_test, y_test, label="Model")
ax.plot(X_test, output(X_test), label="explicit Model", ls=':')
ax.plot(X_test, cel_0(X_test)* rm.coefs_[1][0][0], label=r"$w_0^1$ . cel_0",␣
 ↪ls='--')
ax.plot(X_test, cel_1(X_test)* rm.coefs_[1][1][0], label=r"$w_1^1$ . cel_1",␣
 ↪ls='--')
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).

[18]:
```
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 1.3 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.
```