L12_Neural_Networks_filled

January 25, 2019

In [1]:
```
from keras.models import Sequential
from keras.layers import Dense
from keras.wrappers.scikit_learn import KerasRegressor
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline

%matplotlib inline
```

```
Using TensorFlow backend.
```

Set our random seed so that all computations are deterministic

In [2]:
```
seed = 21899
```

Read in the raw data for the first 100K records of the HCEPDB into a pandas dataframe

In [3]:
```
df = pd.read_csv('https://github.com/UWDIRECT/UWDIRECT.github.io/blob/master/Wi18_conte
df.head()
```

Out[3]:
```
        id                                        SMILES_str   stoich_str  \
0   655365          C1C=CC=C1c1cc2[se]c3c4occc4c4nsnc4c3c2cn1  C18H9N3OSSe
1  1245190  C1C=CC=C1c1cc2[se]c3c(ncc4ccccc34)c2c2=C[SiH2]...  C22H15NSeSi
2    21847  C1C=c2ccc3c4c[nH]cc4c4c5[SiH2]C(=Cc5oc4c3c2=C1...   C24H17NOSi
3    65553   [SiH2]1C=CC2=C1C=C([SiH2]2)C1=Cc2[se]ccc2[SiH2]1  C12H12SeSi3
4   720918       C1C=c2c3ccsc3c3[se]c4cc(oc4c3c2=C1)C1=CC=CC1   C20H12OSSe

       mass       pce       voc         jsc  e_homo_alpha  e_gap_alpha  \
0  394.3151  5.161953  0.867601   91.567575     -5.467601     2.022944
1  400.4135  5.261398  0.504824  160.401549     -5.104824     1.630750
2  363.4903  0.000000  0.000000  197.474780     -4.539526     1.462158
3  319.4448  6.138294  0.630274  149.887545     -5.230274     1.682250
```

```
4  379.3398  1.991366  0.242119  126.581347     -4.842119     1.809439

   e_lumo_alpha                                      tmp_smiles_str
0     -3.444656        C1=CC=C(C1)c1cc2[se]c3c4occc4c4nsnc4c3c2cn1
1     -3.474074  C1=CC=C(C1)c1cc2[se]c3c(ncc4ccccc34)c2c2=C[SiH...
2     -3.077368  C1=CC=C(C1)C1=Cc2oc3c(c2[SiH2]1)c1c[nH]cc1c1cc...
3     -3.548025  C1=CC2=C([SiH2]1)C=C([SiH2]2)C1=Cc2[se]ccc2[Si...
4     -3.032680       C1=CC=C(C1)c1cc2[se]c3c4sccc4c4=CCC=c4c3c2o1
```

Separate out the predictors from the output

```
In [4]: X = df[['mass', 'voc', 'jsc', 'e_homo_alpha', 'e_gap_alpha',
                'e_lumo_alpha']].values
        Y = df[['pce']].values
```

Let's create the test / train split for these data using 80/20. The _pn extension is related to the 'prenormalization' nature of the data.

```
In [5]: X_train_pn, X_test_pn, y_train, y_test = train_test_split(X, Y,
                                                                   test_size=0.20,
                                                                   random_state=seed)
```

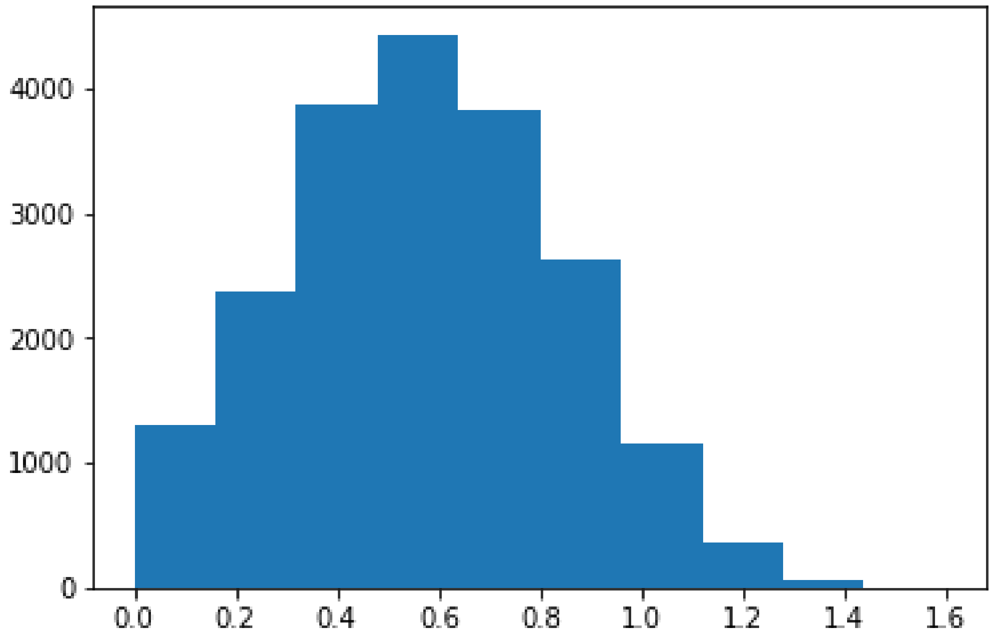
Now we need to StandardScaler the training data and apply that scale to the test data.

```
In [6]: # create the scaler from the training data only and keep it for later use
        X_train_scaler = StandardScaler().fit(X_train_pn)
        # apply the scaler transform to the training data
        X_train = X_train_scaler.transform(X_train_pn)
```

Now let's reuse that scaler transform on the test set. This way we never contaminate the test data with the training data. We'll start with a histogram of the testing data just to prove to ourselves it is working.

```
In [7]: plt.hist(X_test_pn[:,1])

Out[7]: (array([1293., 2369., 3874., 4430., 3822., 2618., 1159.,  359.,   70.,
                   6.]),
         array([0.        , 0.15980339, 0.31960678, 0.47941017, 0.63921356,
                0.79901695, 0.95882034, 1.11862374, 1.27842713, 1.43823052,
                1.59803391]),
         <a list of 10 Patch objects>)
```

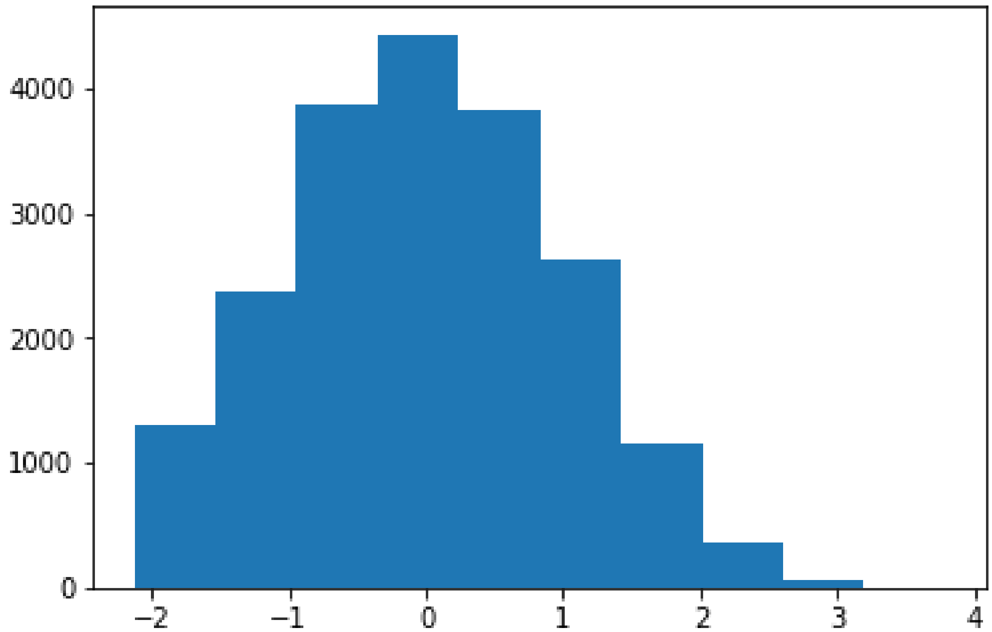


OK, bnow apply the training scaler transform to the test and plot a histogram

```
In [8]: X_test = X_train_scaler.transform(X_test_pn)
```

```
In [9]: plt.hist(X_test[:,1])
```

```
Out[9]: (array([1293., 2369., 3874., 4430., 3822., 2618., 1159.,  359.,   70.,
                   6.]),
         array([-2.12748913, -1.53607743, -0.94466574, -0.35325404,  0.23815766,
                 0.82956935,  1.42098105,  2.01239275,  2.60380444,  3.19521614,
                 3.78662784]),
         <a list of 10 Patch objects>)
```



0.0.1 Let's create the neural network layout

This is a simple neural network with no hidden layers and just the inputs transitioned to the output.

```
In [10]: def simple_model():
             # assemble the structure
             model = Sequential()
             model.add(Dense(6, input_dim=6, kernel_initializer='normal', activation='relu'))
             model.add(Dense(1, kernel_initializer='normal'))
             # compile the model
             model.compile(loss='mean_squared_error', optimizer='adam')
             return model
```

Train the neural network with the following

```
In [11]: # initialize the andom seed as this is used to generate
         # the starting weights
         np.random.seed(seed)
         # create the NN framework
         estimator = KerasRegressor(build_fn=simple_model,
                 epochs=150, batch_size=25000, verbose=0)
         history = estimator.fit(X_train, y_train, validation_split=0.33, epochs=150,
                 batch_size=10000, verbose=0)
```

The history object returned by the `fit` call contains the information in a fitting run.

```
In [12]: print(history.history.keys())
```

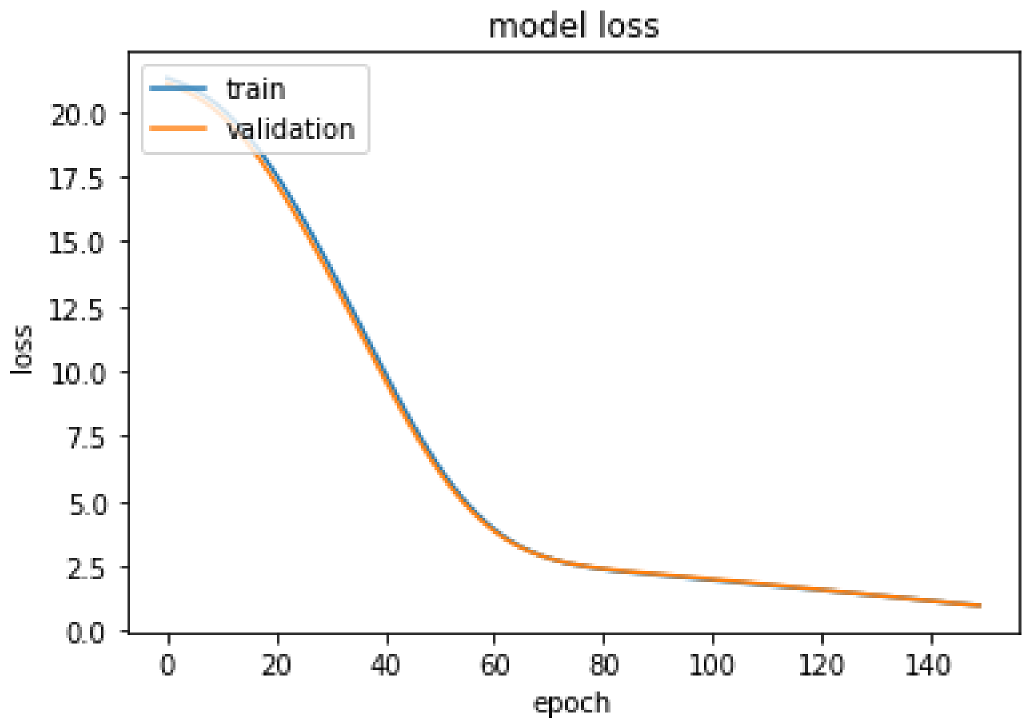
```
dict_keys(['val_loss', 'loss'])
```

```
In [13]: print("final MSE for train is %.2f and for validation is %.2f" %
               (history.history['loss'][-1], history.history['val_loss'][-1]))
```

```
final MSE for train is 0.98 and for validation is 0.98
```

Let's plot it!

```
In [14]: # summarize history for loss
         plt.plot(history.history['loss'])
         plt.plot(history.history['val_loss'])
         plt.title('model loss')
         plt.ylabel('loss')
         plt.xlabel('epoch')
         plt.legend(['train', 'validation'], loc='upper left')
         plt.show()
```



Let's get the MSE for the test set.

```
In [15]: test_loss = estimator.model.evaluate(X_test, y_test)
         print("test set mse is %.2f" % test_loss)
```

```
20000/20000 [==============================] - 1s 26us/step
test set mse is 0.98
```

0.1 NEAT!

So our train mse is very similar to the training and validation at the final step!

0.1.1 Let's look at another way to evaluate the set of models using cross validation

Use 10 fold cross validation to evaluate the models generated from our training set. We'll use scikit-learn's tools for this. Remember, this is only assessing our training set. If you get negative values, to make `cross_val_score` behave as expected, we have to flip the signs on the results (incompatibility with keras).

```
In [16]: kfold = KFold(n_splits=10, random_state=seed)
         results = cross_val_score(estimator, X_train, y_train, cv=kfold)
         print("Results: %.2f (%.2f) MSE" % (-1 * results.mean(), results.std()))
```

```
Results: 3.24 (0.76) MSE
```

Quick aside, `Pipeline` Let's use scikit learns `Pipeline` workflow to run a k-fold cross validation run on the learned model.

With this tool, we create a workflow using the `Pipeline` object. You provide a list of actions (as named tuples) to be performed. We do this with `StandardScaler` to eliminate the posibility of training leakage into the cross validation test set during normalization.

```
In [17]: estimators = []
         estimators.append(('standardize', StandardScaler()))
         estimators.append(('mlp', KerasRegressor(build_fn=simple_model,
                 epochs=150, batch_size=25000, verbose=0)))
         pipeline = Pipeline(estimators)
         kfold = KFold(n_splits=10, random_state=seed)
         results = cross_val_score(pipeline, X_train, y_train, cv=kfold)
         print('MSE mean: %.4f ; std: %.4f' % (-1 * results.mean(), results.std()))
```

```
MSE mean: 3.1070 ; std: 0.4946
```

0.1.2 Now, let's try a more sophisticated model

Let's use a hidden layer this time.

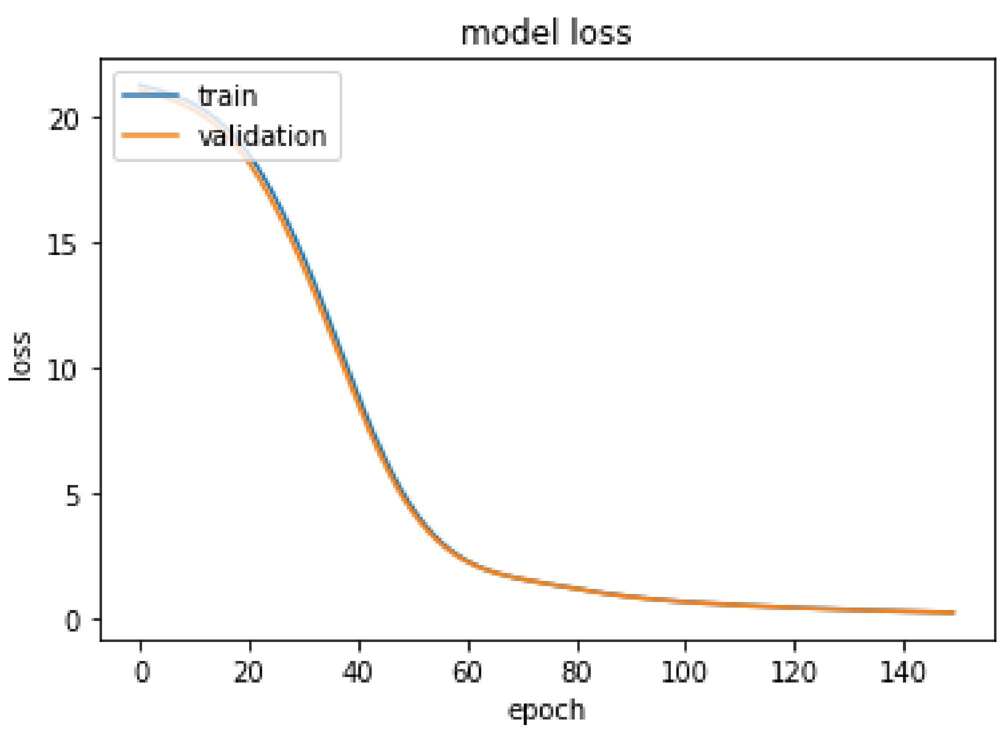
```
In [18]: def medium_model():
             # assemble the structure
             model = Sequential()
             model.add(Dense(6, input_dim=6, kernel_initializer='normal', activation='relu'))
             model.add(Dense(4, kernel_initializer='normal', activation='relu'))
```

```
    model.add(Dense(1, kernel_initializer='normal'))
    # compile the model
    model.compile(loss='mean_squared_error', optimizer='adam')
    return model
```

In [19]:
```
# initialize the andom seed as this is used to generate
# the starting weights
np.random.seed(seed)
# create the NN framework
estimator = KerasRegressor(build_fn=medium_model,
        epochs=150, batch_size=25000, verbose=0)
history = estimator.fit(X_train, y_train, validation_split=0.33, epochs=150,
        batch_size=10000, verbose=0)
print("final MSE for train is %.2f and for validation is %.2f" %
      (history.history['loss'][-1], history.history['val_loss'][-1]))
```

```
final MSE for train is 0.23 and for validation is 0.22
```

In [20]:
```
# summarize history for loss
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('model loss')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['train', 'validation'], loc='upper left')
plt.show()
```



```
In [21]: test_loss = estimator.model.evaluate(X_test, y_test)
         print("test set mse is %.2f" % test_loss)
```

```
20000/20000 [==============================] - 1s 53us/step
test set mse is 0.22
```

So it appears our more complex model improved performance

0.1.3 Free time!

Find example code for keras for the two following items: * L1 and L2 regularization (note in keras, this can be done by layer) * Dropout

Regularization Let's start by adding L1 or L2 (or both) regularization to the hidden layer.

Hint: you need to define a new function that is the neural network model and add the correct parameters to the layer definition. Then retrain and plot as above. What parameters did you choose for your dropout? Did it improve training?

```
In [ ]:
```

```
In [ ]:
```

```
In [ ]:
```

Dropout Find the approach to specifying dropout on a layer using your best friend `bing`. As with L1 and L2 above, this will involve defining a new network struction using a function and some new 'magical' dropout layers.

```
In [ ]:
```

```
In [ ]:
```

```
In [ ]:
```