ex6_sol

May 30, 2018

1 Exercise 6 - Hyperparameter Optimization

This exercise is based on https://github.com/leriomaggio/deep-learning-keras-tensorflow, https://machinelearningmastery.com/grid-search-hyperparameters-deep-learning-models-python-keras/ and https://github.com/fchollet/keras/blob/master/examples/mnist_sklearn_wrapper.py

We want to build simple CNN models to classify the MNIST dataset and uses sklearn's GridSearchCV to find the best hyperparameter model

1.1 Data Preparation

Let's first load and preprocess the data as we did in exercise 5:

```
In [1]: #Import the required libraries
        from keras import backend as K
        import numpy as np
        from keras.utils import np_utils
        from keras.datasets import mnist
        from sklearn.preprocessing import MinMaxScaler
        from sklearn.model_selection import train_test_split

        np.random.seed(1338)  # for reproducibilty!!

        # input image dimensions
        img_rows, img_cols = 28, 28
        # number of classes
        nb_classes = 10

        #Data format
        if K.image_data_format() == 'channels_first':
            shape_ord = (1, img_rows, img_cols)
        else:  # channel_last
            shape_ord = (img_rows, img_cols, 1)

        #Load the data
        (X_train, y_train), (X_test, y_test) = mnist.load_data()
```

```
#Scale the data and concert to data format
scaler = MinMaxScaler(feature_range=(0, 1))
X_train = X_train.astype('float32')
X_test = X_test.astype('float32')
X_train = scaler.fit_transform(X_train.reshape(X_train.shape[0],img_rows*img_cols))
X_test = scaler.transform(X_test.reshape(X_test.shape[0],img_rows*img_cols))
X_train = X_train.reshape(X_train.shape[0],img_rows,img_cols)
X_test = X_test.reshape(X_test.shape[0],img_rows,img_cols)
X_train = X_train.reshape((X_train.shape[0],) + shape_ord)
X_test = X_test.reshape((X_test.shape[0],) + shape_ord)

#convert target vector
Y_train = np_utils.to_categorical(y_train, nb_classes)
Y_test = np_utils.to_categorical(y_test, nb_classes)

#Take just 20k example for training for speed reasons
X_train = X_train[:20000]
Y_train = Y_train[:20000]
```

```
/media/nackenho/Data/programs/ML/anaconda2/lib/python2.7/site-packages/h5py/__init__.py:34: Futu
  from ._conv import register_converters as _register_converters
Using TensorFlow backend.
```

1.2 How to use Keras Models in scikit-learn

Keras models can be used in scikit-learn by wrapping them with the KerasClassifier or KerasRegressor class.

To use these wrappers you must define a function that creates and returns your Keras sequential model, then pass this function to the build_fn argument when constructing the KerasClassifier class.

You can learn more about the scikit-learn wrapper in Keras API documentation: https://keras.io/scikit-learn-api/

1.3 Build Model

We will define a function which builds a similar model we used in exercise 5, but depends on all hyperparameter we would like to tune:

```
In [2]: from keras.models import Sequential
        from keras.layers import Dense, Dropout, Activation, Flatten
        from keras.layers import Conv2D, MaxPooling2D
        from keras.wrappers.scikit_learn import KerasClassifier
```

```
In [3]: def make_model(dense_layer_sizes, dense_activation, filters,
                       kernel_size, pool_size, padding_type, stride_size, dropout_rate, optimize
            '''Creates model comprised of 2 convolutional layers followed by dense layers

            dense_layer_sizes: List of layer sizes. This list has one number for each layer
```

```python
    dense_activation: activation funciton in dense layer
    filters: Number of convolutional filters in each convolutional layer
    kernel_size: Convolutional kernel size
    pool_size: Size of pooling area for max pooling
    padding_type: type of padding: same or valid
    stride_size: symmetric stride size
    dropout_rate: dropout rate
    optimizer: optimizer used for mimizing
    '''

    model = Sequential()

    model.add(Conv2D(filters, (kernel_size, kernel_size), padding=padding_type,
                     strides=(stride_size, stride_size), activation='relu', input_shape=
    model.add(MaxPooling2D(pool_size=(pool_size, pool_size)))
    model.add(Dropout(dropout_rate))
    model.add(Flatten())
    for layer_size in dense_layer_sizes:
        model.add(Dense(layer_size, activation=dense_activation))
    model.add(Dropout(dropout_rate))
    model.add(Dense(nb_classes))
    model.add(Activation('softmax'))

    model.compile(loss='categorical_crossentropy', optimizer=optimizer,metrics=['accurac

    return model
```

```
In [4]: my_cnn = KerasClassifier(make_model)
```

Note: Not even all hyperparameter are included here, we are not varying things like the neural network weight initialization

`model.add(Dense(layer_size, activation=dense_activation, kernel_initializer=init_mode))` with `init_mode = ['uniform', 'lecun_uniform', 'normal', 'zero', 'glorot_normal', 'glorot_uniform', 'he_normal', 'he_uniform']`

or we have not included kernel regularizer like l1/l2 for which we would need to change the strength. The parameter of the optimizer are also not yet included, but we will do that later.

1.4 How to use Grid Search in scikit-learn

Grid search is a model hyperparameter optimization technique. More information on hyperparameter optimization can be found here: http://scikit-learn.org/stable/modules/grid_search.html

In scikit-learn this technique is provided in the `GridSearchCV` class.

When constructing this class you must provide a dictionary of hyperparameters to evaluate in the param_grid argument. This is a map of the model parameter name and an array of values to try.

By default, accuracy is the score that is optimized, but other scores can be specified in the score argument of the GridSearchCV constructor.

By default, the grid search will only use one thread. By setting the n_jobs argument in the GridSearchCV constructor to -1, the process will use all cores on your machine. Depending on your Keras backend, this may interfere with the main neural network training process.

The GridSearchCV process will then construct and evaluate one model for each combination of parameters. Cross validation is used to evaluate each individual model and by default a 3-fold cross validation is used, although this can be overridden by specifying the cv argument to the GridSearchCV constructor. Below is an example of defining a simple grid search:

`param_grid = dict(epochs=[10,20,30])` `grid = GridSearchCV(estimator=model, param_grid=param_grid, n_jobs=-1)` `grid_result = grid.fit(X, Y)`

Once completed, you can access the outcome of the grid search in the result object returned from grid.fit(). The best_score_ member provides access to the best score observed during the optimization procedure and the best_params_ describes the combination of parameters that achieved the best results.

You can learn more about it here:

http://scikit-learn.org/stable/modules/generated/sklearn.grid_search.GridSearchCV.html#sklearn.grid_se

```
In [5]: from sklearn.model_selection import GridSearchCV
```

1.5 GridSearch HyperParameters

First we would like to optimize the convolutional part of the NN, we fix everything else and vary the filter, kernel size, pool size. We could change the padding type and the striding, but we know that padding won't have a large impact, since there is no information in the corners and we neglect striding for now.

```
In [6]: dense_size_candidates = [[32]]
        optimizer = ['Adam']
        activation = ['relu']

        param_grid={'dense_layer_sizes': dense_size_candidates,
                    'dense_activation' : activation,
                     'filters': [16, 32],
                     'kernel_size': [3, 5],
                     'pool_size': [2, 4],
                     'padding_type' : ['valid'],
                     'stride_size'  : [1],
                     'dropout_rate' : [0.5],
                     'optimizer' : optimizer,
                     # epochs and batch_size are avail for tuning even when not
                     # an argument to model building function
                     'epochs': [1],
                     'batch_size': [256]
                      }
```

1.6 ModelCheckpoint

We want to save the best model for each grid search step (we could also save all of them, of course). For that we will use the ModelCheckpoint call back function, which is also useful to save a NN model after each epoch.

```
In [7]: from keras.callbacks import ModelCheckpoint

        filepath = "best_cnn.hdf5"
        checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, mo
```

1.7 Run the grid search

We will use cross-validation with k=2 (speed) and `average precision` as a score value to find the best parameter set. The best metric for optimization depends on your problem, you can find a built-in list here: http://scikit-learn.org/stable/modules/model_evaluation.html#scoring-parameter But you can also define your own scoring function: http://scikit-learn.org/stable/modules/model_evaluation.html#defining-your-scoring-strategy-from-metric-functions

```
In [8]: grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
        grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 2s 232us/step - loss: 1.6526 - acc: 0.4386

Epoch 00001: acc improved from -inf to 0.43860, saving model to best_cnn.hdf5
Epoch 1/1
10000/10000 [==============================] - 2s 227us/step - loss: 1.8641 - acc: 0.3450

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 2s 175us/step - loss: 2.1803 - acc: 0.2091

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 2s 183us/step - loss: 2.1643 - acc: 0.2233

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 3s 289us/step - loss: 1.7412 - acc: 0.4146

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 3s 310us/step - loss: 1.7228 - acc: 0.4009

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 3s 269us/step - loss: 2.1662 - acc: 0.2050

Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 3s 267us/step - loss: 2.2091 - acc: 0.1758
```

```
Epoch 00001: acc did not improve from 0.43860
Epoch 1/1
10000/10000 [==============================] - 4s 365us/step - loss: 1.4888 - acc: 0.5076

Epoch 00001: acc improved from 0.43860 to 0.50760, saving model to best_cnn.hdf5
Epoch 1/1
10000/10000 [==============================] - 4s 394us/step - loss: 1.5462 - acc: 0.4951

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 3s 310us/step - loss: 2.0697 - acc: 0.2831 0s - l

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 3s 298us/step - loss: 2.0067 - acc: 0.2786

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 4s 446us/step - loss: 1.6145 - acc: 0.4447

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 4s 433us/step - loss: 1.4958 - acc: 0.4947

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 5s 515us/step - loss: 1.9818 - acc: 0.3135

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
10000/10000 [==============================] - 4s 448us/step - loss: 1.9938 - acc: 0.2980

Epoch 00001: acc did not improve from 0.50760
Epoch 1/1
20000/20000 [==============================] - 8s 408us/step - loss: 1.1035 - acc: 0.6481

Epoch 00001: acc improved from 0.50760 to 0.64810, saving model to best_cnn.hdf5
```

In [9]:
```python
# summarize results
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
for mean, stdev, param in zip(means, stds, params):
    print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.921226 using {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'valid',
0.897022 (0.013736) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
```

```
0.697076 (0.006241) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.894810 (0.001824) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.704866 (0.000387) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.911370 (0.007887) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.763336 (0.005119) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.921226 (0.001332) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.819737 (0.025760) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
```

1.8 Task 1: Perform a sequentiell grid search to optimze the following hyperparameter. Save the best model for each of the sequentiell steps into a hdf5 file.

- Find the best optimizer: `'SGD', 'RMSprop', 'Adagrad', 'Adadelta', 'Adam', 'Adamax', 'Nadam'`
- Find the best dense structure: Change the width and the depth and try at least 4 different structures
- Find the best activation function for the dense network `'softmax', 'softplus', 'softsign', 'relu', 'tanh', 'sigmoid', 'hard_sigmoid', 'linear'`
- Find the best dropout rate: Change dropout between 0 and 0.5 in 0.1 steps
- Find the best optimizer parameter: In order to do that, you need to change the make_model function to adapt for that. Vary the parameter in a meaningful range.

1.9 Change the optimizer

In [10]:
```python
optimizer = ['SGD', 'RMSprop', 'Adagrad', 'Adadelta', 'Adam', 'Adamax', 'Nadam']
param_grid={'dense_layer_sizes': dense_size_candidates,
             'dense_activation' : activation,
              'filters': [32],
              'kernel_size': [5],
              'pool_size': [2],
              'padding_type' : ['valid'],
              'stride_size'  : [1],
              'dropout_rate' : [0.5],
              'optimizer' : optimizer,
              # epochs and batch_size are avail for tuning even when not
              # an argument to model building function
              'epochs': [1],
              'batch_size': [256]
               }
```

In [11]:
```python
filepath = "best_optimizer.hdf5"
checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, m

grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 4s 441us/step - loss: 2.2812 - acc: 0.1367
```

```
Epoch 00001: acc improved from -inf to 0.13670, saving model to best_optimizer.hdf5
Epoch 1/1
10000/10000 [==============================] - 4s 438us/step - loss: 2.2716 - acc: 0.1514

Epoch 00001: acc improved from 0.13670 to 0.15140, saving model to best_optimizer.hdf5
Epoch 1/1
10000/10000 [==============================] - 9s 896us/step - loss: 1.4214 - acc: 0.5328

Epoch 00001: acc improved from 0.15140 to 0.53280, saving model to best_optimizer.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 624us/step - loss: 1.4039 - acc: 0.5428

Epoch 00001: acc improved from 0.53280 to 0.54280, saving model to best_optimizer.hdf5
Epoch 1/1
10000/10000 [==============================] - 5s 519us/step - loss: 1.1625 - acc: 0.6008

Epoch 00001: acc improved from 0.54280 to 0.60080, saving model to best_optimizer.hdf5
Epoch 1/1
10000/10000 [==============================] - 7s 685us/step - loss: 1.2064 - acc: 0.5855

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 6s 584us/step - loss: 1.4104 - acc: 0.5274

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 6s 618us/step - loss: 1.5349 - acc: 0.4924

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 5s 528us/step - loss: 1.4916 - acc: 0.4935

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 7s 726us/step - loss: 1.4825 - acc: 0.4892

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 7s 661us/step - loss: 1.5640 - acc: 0.4703

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 5s 545us/step - loss: 1.4340 - acc: 0.5162

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 8s 781us/step - loss: 1.3129 - acc: 0.5536
```

```
Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
10000/10000 [==============================] - 7s 708us/step - loss: 1.2689 - acc: 0.5847

Epoch 00001: acc did not improve from 0.60080
Epoch 1/1
20000/20000 [==============================] - 14s 688us/step - loss: 0.7952 - acc: 0.7385

Epoch 00001: acc improved from 0.60080 to 0.73855, saving model to best_optimizer.hdf5
```

```
In [12]: # summarize results
         print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
         means = grid_result.cv_results_['mean_test_score']
         stds = grid_result.cv_results_['std_test_score']
         params = grid_result.cv_results_['params']
         for mean, stdev, param in zip(means, stds, params):
             print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.953131 using {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'valid',
0.432478 (0.031058) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.919020 (0.007165) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.953131 (0.003355) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.917285 (0.007868) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.921445 (0.016463) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.920814 (0.000985) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.944096 (0.002705) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
```

1.10 Change the dense structure

```
In [13]: optimizer = ['Adagrad']
         dense_size_candidates = [[32], [64], [32, 32], [64, 64]]

         param_grid={'dense_layer_sizes': dense_size_candidates,
                     'dense_activation' : activation,
                      'filters': [32],
                      'kernel_size': [5],
                      'pool_size': [2],
                      'padding_type' : ['valid'],
                      'stride_size'  : [1],
                      'dropout_rate' : [0.5],
                      'optimizer' : optimizer,
                      # epochs and batch_size are avail for tuning even when not
                      # an argument to model building function
                      'epochs': [1],
                      'batch_size': [256]
                    }
```

```
In [14]: filepath = "best_dnnstruc.hdf5"
         checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, m

         grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
         grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 6s 587us/step - loss: 1.1246 - acc: 0.6261

Epoch 00001: acc improved from -inf to 0.62610, saving model to best_dnnstruc.hdf5
Epoch 1/1
10000/10000 [==============================] - 5s 524us/step - loss: 1.2111 - acc: 0.5962

Epoch 00001: acc did not improve from 0.62610
Epoch 1/1
10000/10000 [==============================] - 6s 565us/step - loss: 0.8494 - acc: 0.7286

Epoch 00001: acc improved from 0.62610 to 0.72860, saving model to best_dnnstruc.hdf5
Epoch 1/1
10000/10000 [==============================] - 7s 683us/step - loss: 1.0527 - acc: 0.6630

Epoch 00001: acc did not improve from 0.72860
Epoch 1/1
10000/10000 [==============================] - 6s 627us/step - loss: 1.3466 - acc: 0.5412

Epoch 00001: acc did not improve from 0.72860
Epoch 1/1
10000/10000 [==============================] - 6s 565us/step - loss: 1.3039 - acc: 0.5483 3s - l

Epoch 00001: acc did not improve from 0.72860
Epoch 1/1
10000/10000 [==============================] - 7s 701us/step - loss: 1.0811 - acc: 0.6498

Epoch 00001: acc did not improve from 0.72860
Epoch 1/1
10000/10000 [==============================] - 6s 584us/step - loss: 0.9778 - acc: 0.6871

Epoch 00001: acc did not improve from 0.72860
Epoch 1/1
20000/20000 [==============================] - 10s 524us/step - loss: 0.6282 - acc: 0.8069

Epoch 00001: acc improved from 0.72860 to 0.80695, saving model to best_dnnstruc.hdf5
```

```
In [15]: # summarize results
         print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
         means = grid_result.cv_results_['mean_test_score']
         stds = grid_result.cv_results_['std_test_score']
```

```
params = grid_result.cv_results_['params']
for mean, stdev, param in zip(means, stds, params):
    print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.972087 using {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'valid',
0.954223 (0.001573) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.972087 (0.003852) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.948875 (0.001103) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.966096 (0.000288) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
```

1.11 Change the dense activation

In [16]:
```
optimizer = ['Adagrad']
dense_size_candidates = [[64]]
activation = ['softmax', 'softplus', 'softsign', 'relu', 'tanh', 'sigmoid', 'hard_sigmo

param_grid={'dense_layer_sizes': dense_size_candidates,
            'dense_activation' : activation,
             'filters': [32],
             'kernel_size': [5],
             'pool_size': [2],
             'padding_type' : ['valid'],
             'stride_size'  : [1],
             'dropout_rate' : [0.5],
             'optimizer' : optimizer,
             # epochs and batch_size are avail for tuning even when not
             # an argument to model building function
             'epochs': [1],
             'batch_size': [256]
              }
```

In [17]:
```
filepath = "best_dnnact.hdf5"
checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, m

grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 6s 575us/step - loss: 2.0666 - acc: 0.3660

Epoch 00001: acc improved from -inf to 0.36600, saving model to best_dnnact.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 585us/step - loss: 2.0557 - acc: 0.4155

Epoch 00001: acc improved from 0.36600 to 0.41550, saving model to best_dnnact.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 600us/step - loss: 0.9658 - acc: 0.6856
```

```
Epoch 00001: acc improved from 0.41550 to 0.68560, saving model to best_dnnact.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 569us/step - loss: 1.0423 - acc: 0.6630

Epoch 00001: acc did not improve from 0.68560
Epoch 1/1
10000/10000 [==============================] - 6s 648us/step - loss: 0.7227 - acc: 0.7942

Epoch 00001: acc improved from 0.68560 to 0.79420, saving model to best_dnnact.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 616us/step - loss: 0.7807 - acc: 0.7758

Epoch 00001: acc did not improve from 0.79420
Epoch 1/1
10000/10000 [==============================] - 6s 596us/step - loss: 0.8795 - acc: 0.7177

Epoch 00001: acc did not improve from 0.79420
Epoch 1/1
10000/10000 [==============================] - 7s 747us/step - loss: 0.9175 - acc: 0.7156

Epoch 00001: acc did not improve from 0.79420
Epoch 1/1
10000/10000 [==============================] - 6s 645us/step - loss: 0.6806 - acc: 0.7942

Epoch 00001: acc did not improve from 0.79420
Epoch 1/1
10000/10000 [==============================] - 7s 685us/step - loss: 0.6926 - acc: 0.7971

Epoch 00001: acc improved from 0.79420 to 0.79710, saving model to best_dnnact.hdf5
Epoch 1/1
10000/10000 [==============================] - 7s 658us/step - loss: 1.0615 - acc: 0.6912

Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
10000/10000 [==============================] - 6s 577us/step - loss: 1.0707 - acc: 0.6945

Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
10000/10000 [==============================] - 7s 665us/step - loss: 1.0372 - acc: 0.7043

Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
10000/10000 [==============================] - 7s 667us/step - loss: 0.9995 - acc: 0.7059

Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
10000/10000 [==============================] - 7s 656us/step - loss: 0.7255 - acc: 0.7774
```

```
Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
10000/10000 [==============================] - 6s 613us/step - loss: 0.8233 - acc: 0.7699

Epoch 00001: acc did not improve from 0.79710
Epoch 1/1
20000/20000 [==============================] - 11s 572us/step - loss: 0.6938 - acc: 0.7849

Epoch 00001: acc did not improve from 0.79710
```

```
In [18]: # summarize results
         print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
         means = grid_result.cv_results_['mean_test_score']
         stds = grid_result.cv_results_['std_test_score']
         params = grid_result.cv_results_['params']
         for mean, stdev, param in zip(means, stds, params):
             print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.975186 using {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'valid',
0.798972 (0.016352) with: {'dropout_rate': 0.5, 'dense_activation': 'softmax', 'padding_type': '
0.960227 (0.003834) with: {'dropout_rate': 0.5, 'dense_activation': 'softplus', 'padding_type':
0.972510 (0.002323) with: {'dropout_rate': 0.5, 'dense_activation': 'softsign', 'padding_type':
0.975186 (0.000084) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
0.973520 (0.004743) with: {'dropout_rate': 0.5, 'dense_activation': 'tanh', 'padding_type': 'val
0.954002 (0.003930) with: {'dropout_rate': 0.5, 'dense_activation': 'sigmoid', 'padding_type': '
0.955399 (0.008666) with: {'dropout_rate': 0.5, 'dense_activation': 'hard_sigmoid', 'padding_typ
0.972284 (0.004204) with: {'dropout_rate': 0.5, 'dense_activation': 'linear', 'padding_type': 'v
```

1.12 Change the dropout rate

```
In [19]: optimizer = ['Adagrad']
         dense_size_candidates = [[64]]
         activation = ['relu']

         param_grid={'dense_layer_sizes': dense_size_candidates,
                     'dense_activation' : activation,
                      'filters': [32],
                      'kernel_size': [5],
                      'pool_size': [2],
                      'padding_type' : ['valid'],
                      'stride_size'  : [1],
                      'dropout_rate' : [0.1, 0.2, 0.3, 0.4, 0.5],
                      'optimizer' : optimizer,
                      # epochs and batch_size are avail for tuning even when not
                      # an argument to model building function
                      'epochs': [1],
```

```
                    'batch_size': [256]
                     }
```

```
In [20]: filepath = "best_dropout.hdf5"
         checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, m

         grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
         grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 7s 699us/step - loss: 0.7614 - acc: 0.7725

Epoch 00001: acc improved from -inf to 0.77250, saving model to best_dropout.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 640us/step - loss: 0.7525 - acc: 0.7619

Epoch 00001: acc did not improve from 0.77250
Epoch 1/1
10000/10000 [==============================] - 6s 619us/step - loss: 0.6616 - acc: 0.7915

Epoch 00001: acc improved from 0.77250 to 0.79150, saving model to best_dropout.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 615us/step - loss: 0.7723 - acc: 0.7703

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 7s 665us/step - loss: 0.7761 - acc: 0.7571

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 6s 614us/step - loss: 0.7375 - acc: 0.7693

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 7s 686us/step - loss: 0.8288 - acc: 0.7365

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 6s 615us/step - loss: 0.9020 - acc: 0.7219

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 6s 585us/step - loss: 0.9584 - acc: 0.6959

Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
10000/10000 [==============================] - 7s 732us/step - loss: 0.8572 - acc: 0.7317
```

```
Epoch 00001: acc did not improve from 0.79150
Epoch 1/1
20000/20000 [==============================] - 22s 1ms/step - loss: 0.5069 - acc: 0.8514

Epoch 00001: acc improved from 0.79150 to 0.85135, saving model to best_dropout.hdf5
```

```
In [21]: # summarize results
         print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
         means = grid_result.cv_results_['mean_test_score']
         stds = grid_result.cv_results_['std_test_score']
         params = grid_result.cv_results_['params']
         for mean, stdev, param in zip(means, stds, params):
             print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.975560 using {'dropout_rate': 0.2, 'dense_activation': 'relu', 'padding_type': 'valid',
0.962235 (0.000827) with: {'dropout_rate': 0.1, 'dense_activation': 'relu', 'padding_type': 'val
0.975560 (0.004739) with: {'dropout_rate': 0.2, 'dense_activation': 'relu', 'padding_type': 'val
0.970889 (0.001845) with: {'dropout_rate': 0.3, 'dense_activation': 'relu', 'padding_type': 'val
0.940339 (0.030595) with: {'dropout_rate': 0.4, 'dense_activation': 'relu', 'padding_type': 'val
0.974625 (0.000511) with: {'dropout_rate': 0.5, 'dense_activation': 'relu', 'padding_type': 'val
```

1.13 Change the optimizer parameter

```
In [22]: from keras.optimizers import Adam

         def make_model(dense_layer_sizes, dense_activation, filters,
                        kernel_size, pool_size, padding_type, stride_size, dropout_rate, learn_r
             '''Creates model comprised of 2 convolutional layers followed by dense layers

             dense_layer_sizes: List of layer sizes. This list has one number for each layer
             dense_activation: activation funciton in dense layer
             filters: Number of convolutional filters in each convolutional layer
             kernel_size: Convolutional kernel size
             pool_size: Size of pooling area for max pooling
             padding_type: type of padding: same or valid
             stride_size: symmetric stride size
             dropout_rate: dropout rate
             optimizer: optimizer used for mimizing
             '''

             optimizer = Adam(lr=learn_rate, beta_1=beta_1, beta_2=beta_2, decay=decay)

             model = Sequential()

             model.add(Conv2D(filters, (kernel_size, kernel_size), padding=padding_type,
                              strides=(stride_size, stride_size), activation='relu', input_shape
```

```
            model.add(MaxPooling2D(pool_size=(pool_size, pool_size)))
            model.add(Dropout(dropout_rate))
            model.add(Flatten())
            for layer_size in dense_layer_sizes:
                model.add(Dense(layer_size, activation=dense_activation))
            model.add(Dropout(dropout_rate))
            model.add(Dense(nb_classes))
            model.add(Activation('softmax'))

            model.compile(loss='categorical_crossentropy', optimizer=optimizer,metrics=['accura

            return model

        my_cnn = KerasClassifier(make_model)
```

In [23]:
```
dense_size_candidates = [[64]]
activation = ['relu']

param_grid={'dense_layer_sizes': dense_size_candidates,
            'dense_activation' : activation,
             'filters': [32],
             'kernel_size': [5],
             'pool_size': [2],
             'padding_type' : ['valid'],
             'stride_size'  : [1],
             'dropout_rate' : [0.2],
             # epochs and batch_size are avail for tuning even when not
             # an argument to model building function
             'epochs': [1],
             'batch_size': [256],
             'learn_rate' : [0.001, 0.0001],
             'beta_1' : [0.9, 0.8],
             'beta_2' : [0.999],
             'decay'  : [0.0, 0.3]

              }
```

In [24]:
```
filepath = "best_adampar.hdf5"
checkpoint = ModelCheckpoint(filepath, monitor='acc', verbose=1, save_best_only=True, m

grid = GridSearchCV(my_cnn, param_grid, cv=2, scoring='average_precision', n_jobs=1)
grid_result = grid.fit(X_train, Y_train, callbacks=[checkpoint])
```

```
Epoch 1/1
10000/10000 [==============================] - 6s 608us/step - loss: 0.9922 - acc: 0.7063

Epoch 00001: acc improved from -inf to 0.70630, saving model to best_adampar.hdf5
Epoch 1/1
```

```
10000/10000 [==============================] - 6s 629us/step - loss: 0.9303 - acc: 0.7235

Epoch 00001: acc improved from 0.70630 to 0.72350, saving model to best_adampar.hdf5
Epoch 1/1
10000/10000 [==============================] - 8s 788us/step - loss: 2.0841 - acc: 0.4044

Epoch 00001: acc did not improve from 0.72350
Epoch 1/1
10000/10000 [==============================] - 7s 746us/step - loss: 2.1117 - acc: 0.4060

Epoch 00001: acc did not improve from 0.72350
WARNING:tensorflow:Variable *= will be deprecated. Use variable.assign_mul if you want assignmen
Epoch 1/1
10000/10000 [==============================] - 9s 902us/step - loss: 1.6133 - acc: 0.5807

Epoch 00001: acc did not improve from 0.72350
Epoch 1/1
10000/10000 [==============================] - 7s 678us/step - loss: 1.5931 - acc: 0.6310

Epoch 00001: acc did not improve from 0.72350
Epoch 1/1
10000/10000 [==============================] - 8s 802us/step - loss: 2.2535 - acc: 0.2326

Epoch 00001: acc did not improve from 0.72350
Epoch 1/1
10000/10000 [==============================] - 7s 738us/step - loss: 2.2317 - acc: 0.2175 3s - l

Epoch 00001: acc did not improve from 0.72350
Epoch 1/1
10000/10000 [==============================] - 6s 640us/step - loss: 0.9763 - acc: 0.7257

Epoch 00001: acc improved from 0.72350 to 0.72570, saving model to best_adampar.hdf5
Epoch 1/1
10000/10000 [==============================] - 6s 610us/step - loss: 0.9176 - acc: 0.7310

Epoch 00001: acc improved from 0.72570 to 0.73100, saving model to best_adampar.hdf5
Epoch 1/1
10000/10000 [==============================] - 7s 656us/step - loss: 2.0361 - acc: 0.3800

Epoch 00001: acc did not improve from 0.73100
Epoch 1/1
10000/10000 [==============================] - 7s 692us/step - loss: 2.0357 - acc: 0.3764

Epoch 00001: acc did not improve from 0.73100
Epoch 1/1
10000/10000 [==============================] - 8s 843us/step - loss: 1.5357 - acc: 0.6266

Epoch 00001: acc did not improve from 0.73100
```

```
Epoch 1/1
10000/10000 [==============================] - 10s 1ms/step - loss: 1.5317 - acc: 0.6296

Epoch 00001: acc did not improve from 0.73100
Epoch 1/1
10000/10000 [==============================] - 8s 779us/step - loss: 2.1705 - acc: 0.2692

Epoch 00001: acc did not improve from 0.73100
Epoch 1/1
10000/10000 [==============================] - 7s 745us/step - loss: 2.2333 - acc: 0.2213

Epoch 00001: acc did not improve from 0.73100
Epoch 1/1
20000/20000 [==============================] - 13s 626us/step - loss: 0.6922 - acc: 0.7983

Epoch 00001: acc improved from 0.73100 to 0.79830, saving model to best_adampar.hdf5
```

```
In [25]: # summarize results
         print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
         means = grid_result.cv_results_['mean_test_score']
         stds = grid_result.cv_results_['std_test_score']
         params = grid_result.cv_results_['params']
         for mean, stdev, param in zip(means, stds, params):
             print("%f (%f) with: %r" % (mean, stdev, param))
```

```
Best: 0.956970 using {'beta_1': 0.8, 'learn_rate': 0.001, 'dropout_rate': 0.2, 'beta_2': 0.999,
0.953437 (0.001145) with: {'beta_1': 0.9, 'learn_rate': 0.001, 'dropout_rate': 0.2, 'beta_2': 0.
0.812760 (0.012938) with: {'beta_1': 0.9, 'learn_rate': 0.0001, 'dropout_rate': 0.2, 'beta_2': 0
0.866507 (0.001715) with: {'beta_1': 0.9, 'learn_rate': 0.001, 'dropout_rate': 0.2, 'beta_2': 0.
0.478708 (0.014245) with: {'beta_1': 0.9, 'learn_rate': 0.0001, 'dropout_rate': 0.2, 'beta_2': 0
0.956970 (0.002731) with: {'beta_1': 0.8, 'learn_rate': 0.001, 'dropout_rate': 0.2, 'beta_2': 0.
0.808314 (0.022256) with: {'beta_1': 0.8, 'learn_rate': 0.0001, 'dropout_rate': 0.2, 'beta_2': 0
0.880496 (0.007163) with: {'beta_1': 0.8, 'learn_rate': 0.001, 'dropout_rate': 0.2, 'beta_2': 0.
0.517567 (0.011910) with: {'beta_1': 0.8, 'learn_rate': 0.0001, 'dropout_rate': 0.2, 'beta_2': 0
```

1.14 Tips for Hyperparameter Optimization

This section lists some handy tips to consider when tuning hyperparameters of your neural network.

- **k-fold Cross Validation.** You can see that the results from the examples in this post show some variance. For speed reasons, we used a cross-validation of 2, but perhaps k=5 or k=10 would be more stable. Carefully choose your cross validation configuration to ensure your results are stable.
- **Review the Whole Grid.** Do not just focus on the best result, review the whole grid of results and look for trends to support configuration decisions.

- **Parallelize.** Use all your cores if you can, neural networks are slow to train and we often want to try a lot of different parameters. Consider using cluster instances if available.
- **Use a Sample of Your Dataset.** Because networks are slow to train, try training them on a smaller sample of your training dataset, just to get an idea of general directions of parameters rather than optimal configurations.
- **Start with Coarse Grids.** Start with coarse-grained grids and zoom into finer grained grids once you can narrow the scope.
- **Do not Transfer Results.** Results are generally problem specific. Try to avoid favorite configurations on each new problem that you see. It is unlikely that optimal results you discover on one problem will transfer to your next project. Instead look for broader trends like number of layers or relationships between parameters.
- **Reproducibility is a Problem.** Although we set the seed for the random number generator in NumPy, the results are not 100% reproducible. There is more to reproducibility when grid searching wrapped Keras models than is presented in this post.

1.15 Task 2: Load the best model and evaluate it using the function below

You can load the model using `from keras.models import load_model` `model=load_model('filename')`

```
In [26]: ##########################################################################################

         import matplotlib.pyplot as plt
         %matplotlib inline

         def plot_history(network_history):
             plt.figure()
             plt.xlabel('Epochs')
             plt.ylabel('Loss')
             plt.plot(network_history.history['loss'])
             plt.plot(network_history.history['val_loss'])
             plt.legend(['Training', 'Validation'])

             plt.figure()
             plt.xlabel('Epochs')
             plt.ylabel('Accuracy')
             plt.plot(network_history.history['acc'])
             plt.plot(network_history.history['val_acc'])
             plt.legend(['Training', 'Validation'], loc='lower right')
             plt.show()

         ##########################################################################################

         import itertools
         def plot_confusion_matrix(cm, classes,
                                   normalize=False,
                                   title='Confusion matrix',
                                   cmap=plt.cm.Blues):
```

```
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    plt.imshow(cm, interpolation='nearest', cmap=cmap)
    plt.title(title)
    plt.colorbar()
    tick_marks = np.arange(len(classes))
    plt.xticks(tick_marks, classes, rotation=45)
    plt.yticks(tick_marks, classes)

    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]

    thresh = cm.max() / 2.
    for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
        plt.text(j, i, cm[i, j],
                 horizontalalignment="center",
                 color="white" if cm[i, j] > thresh else "black")

    plt.tight_layout()
    plt.ylabel('True label')
    plt.xlabel('Predicted label')

################################################################################
import matplotlib.cm as cm
def display_errors(errors_index,img_errors,pred_errors, obs_errors):
    """ This function shows 6 images with their predicted and real labels"""
    n = 0
    nrows = 2
    ncols = 3
    fig, ax = plt.subplots(nrows,ncols,sharex=True,sharey=True)
    for row in range(nrows):
        for col in range(ncols):
            error = errors_index[n]
            ax[row,col].imshow((img_errors[error]).reshape((28,28)), cmap=cm.Greys, int
            ax[row,col].set_title("Predicted label :{}\nTrue label :{}".format(pred_err
            n += 1

################################################################################
from sklearn.metrics import confusion_matrix,classification_report

def evaluate(X_test, Y_test, model):

    ##Evaluate loss and metrics
    loss, accuracy = model.evaluate(X_test, Y_test, verbose=0)
    print('Test Loss:', loss)
    print('Test Accuracy:', accuracy)
```

```
# Predict the values from the test dataset
Y_pred = model.predict(X_test)
# Convert predictions classes to one hot vectors
Y_cls = np.argmax(Y_pred, axis = 1)
# Convert validation observations to one hot vectors
Y_true = np.argmax(Y_test, axis = 1)
print 'Classification Report:\n', classification_report(Y_true,Y_cls)

## Plot 0 probability including overtraining test
plt.figure(figsize=(8,8))

label=0
#Test prediction
Y_pred_prob = Y_pred[:,label]
plt.hist(Y_pred_prob[Y_true == label], alpha=0.5, color='red', range=[0, 1], bins=1
plt.hist(Y_pred_prob[Y_true != label], alpha=0.5, color='blue', range=[0, 1], bins=
#Train prediction
Y_train_pred = model.predict(X_train)
Y_train_pred_prob = Y_train_pred[:,label]
Y_train_true = np.argmax(Y_train, axis = 1)
plt.hist(Y_train_pred_prob[Y_train_true == label], alpha=0.5, color='red', range=[0
plt.hist(Y_train_pred_prob[Y_train_true != label], alpha=0.5, color='blue', range=[

plt.legend(['train == 0', 'train != 0', 'test == 0', 'test != 0'], loc='upper right
plt.xlabel('Probability of being 0')
plt.ylabel('Number of entries')
plt.show()

# compute the confusion matrix
confusion_mtx = confusion_matrix(Y_true, Y_cls)
# plot the confusion matrix
plt.figure(figsize=(8,8))
plot_confusion_matrix(confusion_mtx, classes = range(10))

#Plot largest errors
errors = (Y_cls - Y_true != 0)
Y_cls_errors = Y_cls[errors]
Y_pred_errors = Y_pred[errors]
Y_true_errors = Y_true[errors]
X_test_errors = X_test[errors]
# Probabilities of the wrong predicted numbers
Y_pred_errors_prob = np.max(Y_pred_errors,axis = 1)
# Predicted probabilities of the true values in the error set
true_prob_errors = np.diagonal(np.take(Y_pred_errors, Y_true_errors, axis=1))
# Difference between the probability of the predicted label and the true label
delta_pred_true_errors = Y_pred_errors_prob - true_prob_errors
# Sorted list of the delta prob errors
sorted_dela_errors = np.argsort(delta_pred_true_errors)
```

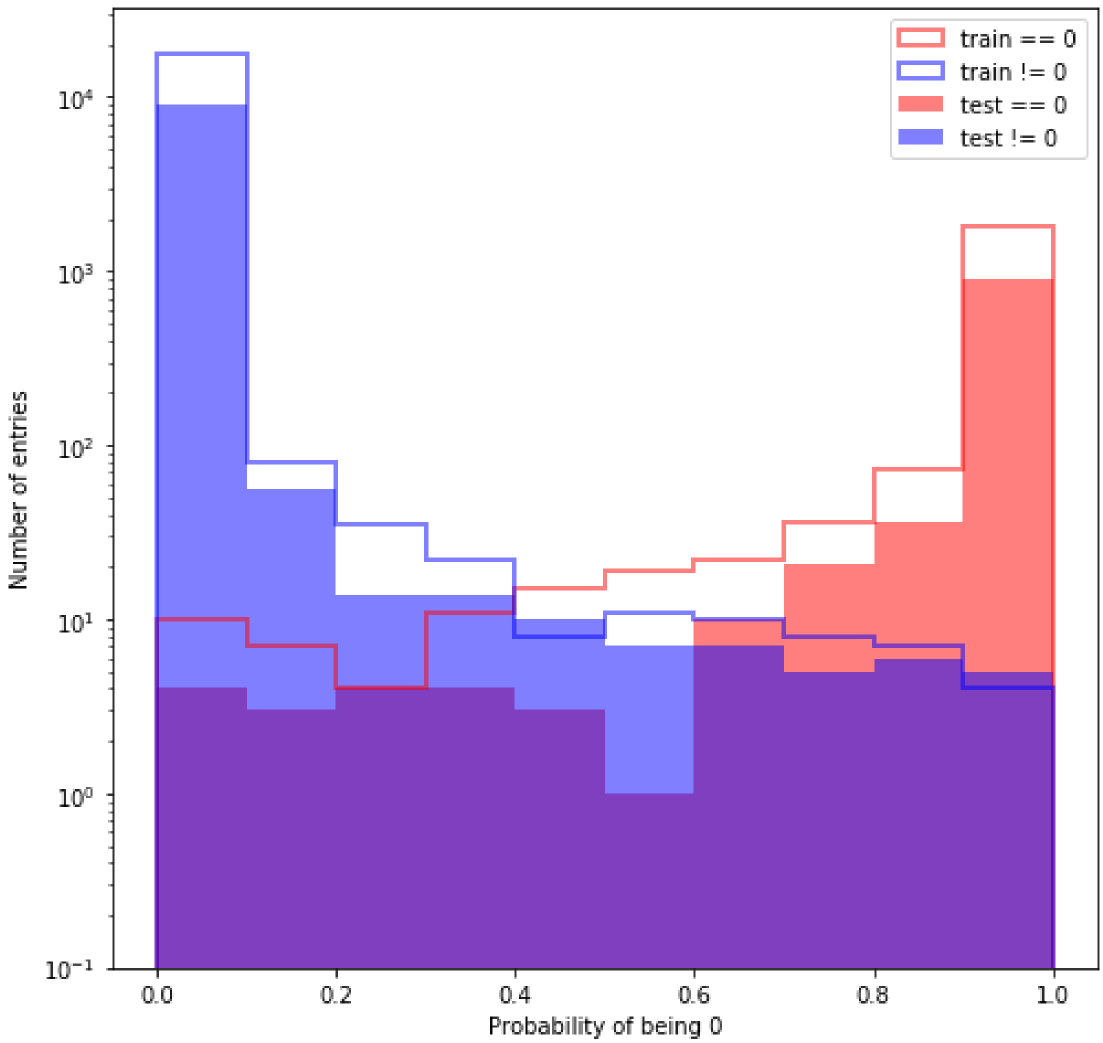
```
# Top 6 errors
most_important_errors = sorted_dela_errors[-6:]
# Show the top 6 errors
display_errors(most_important_errors, X_test_errors, Y_cls_errors, Y_true_errors)

##Plot predictions
slice = 15
predicted = model.predict(X_test[:slice]).argmax(-1)
plt.figure(figsize=(16,8))
for i in range(slice):
    plt.subplot(1, slice, i+1)
    plt.imshow(X_test[i].reshape(28,28), interpolation='nearest')
    plt.text(0, 0, predicted[i], color='black',
             bbox=dict(facecolor='white', alpha=1))
    plt.axis('off')
```

1.16 Load best model and evaluate

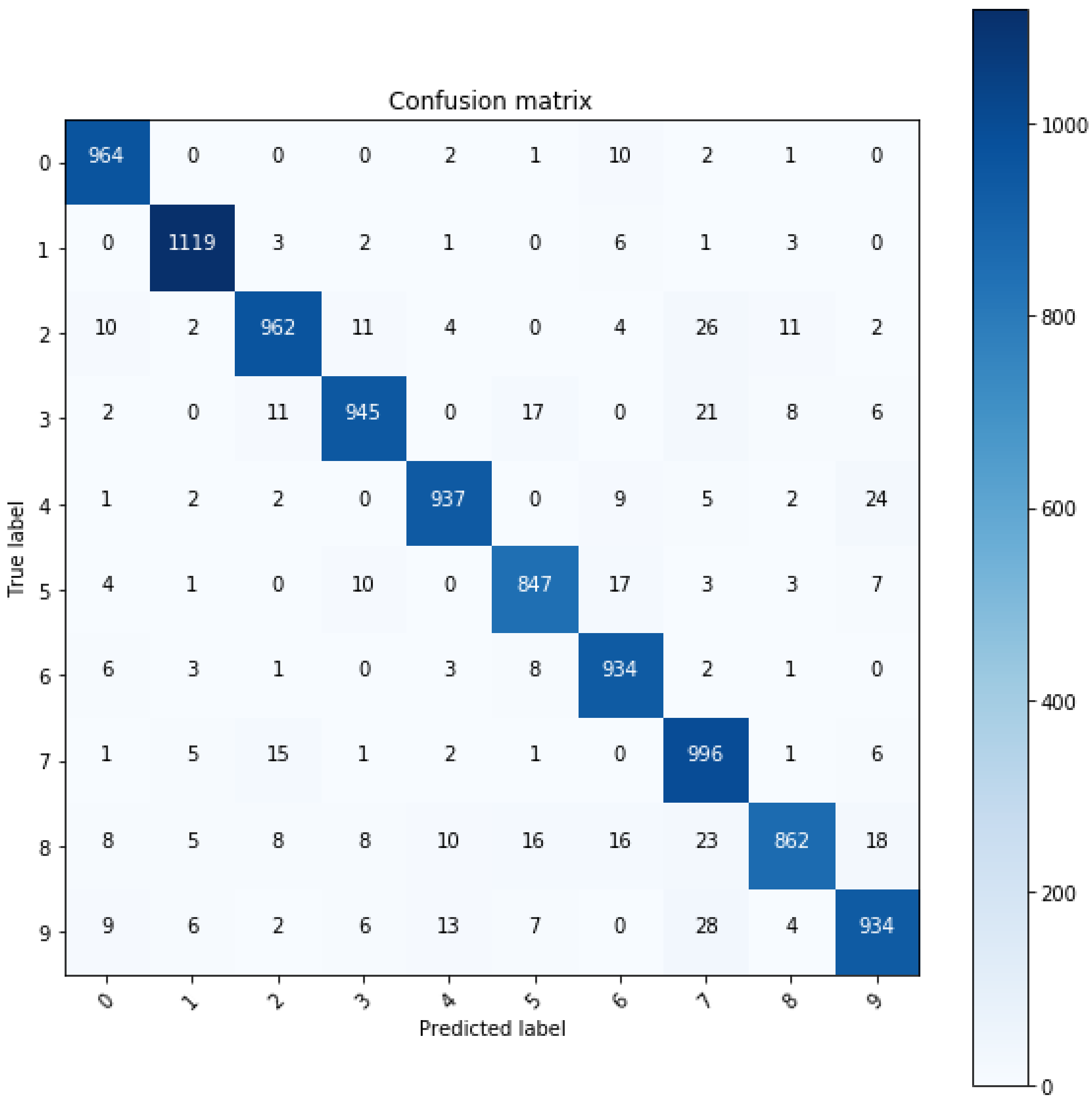
```
In [27]: from keras.models import load_model
         model= load_model('best_dropout.hdf5')
```

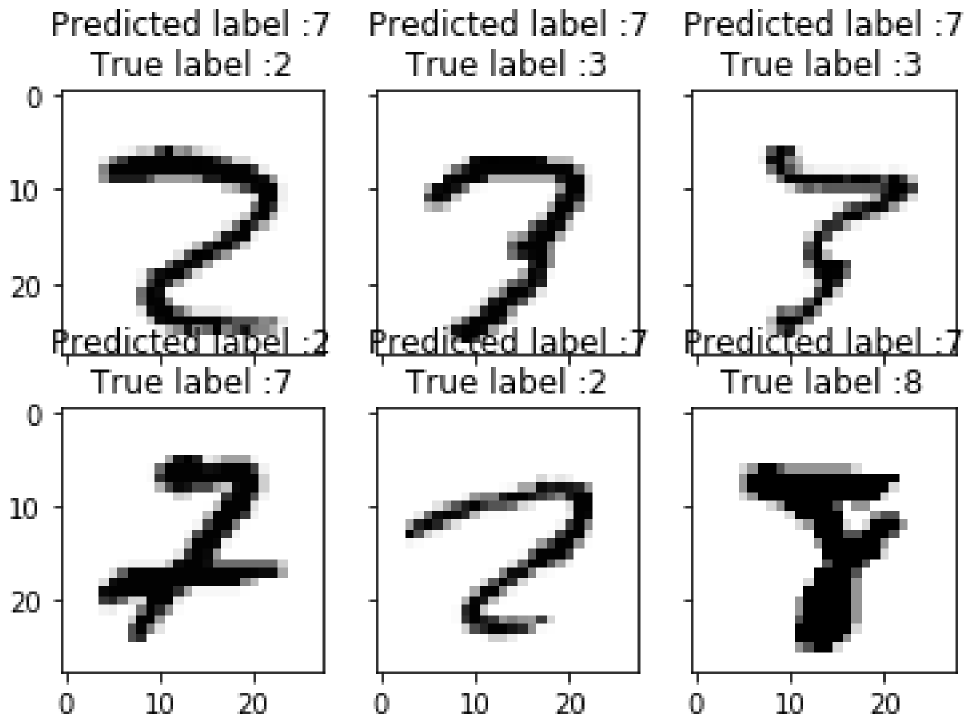
```
In [28]: evaluate(X_test, Y_test, model)
```

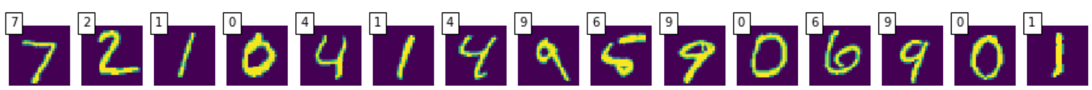
```
('Test Loss:', 0.1721801412165165)
('Test Accuracy:', 0.95)
Classification Report:
             precision    recall  f1-score   support

          0       0.96      0.98      0.97       980
          1       0.98      0.99      0.98      1135
          2       0.96      0.93      0.94      1032
          3       0.96      0.94      0.95      1010
          4       0.96      0.95      0.96       982
          5       0.94      0.95      0.95       892
          6       0.94      0.97      0.96       958
          7       0.90      0.97      0.93      1028
          8       0.96      0.89      0.92       974
          9       0.94      0.93      0.93      1009

avg / total       0.95      0.95      0.95     10000
```



train == 0
train != 0
test == 0
test != 0
Number of entries
Probability of being 0


Confusion matrix
True label
Predicted label
964 0 0 0 2 1 10 2 1 0
0 1119 3 2 1 0 6 1 3 0
10 2 962 11 4 0 4 26 11 2
2 0 11 945 0 17 0 21 8 6
1 2 2 0 937 0 9 5 2 24
4 1 0 10 0 847 17 3 3 7
6 3 1 0 3 8 934 2 1 0
1 5 15 1 2 1 0 996 1 6
8 5 8 8 10 16 16 23 862 18
9 6 2 6 13 7 0 28 4 934
0 1 2 3 4 5 6 7 8 9
1000
800
600
400
200
0





---

2 There's more:

The `GridSearchCV` model in scikit-learn performs a complete search, considering **all** the possible combinations of Hyper-parameters we want to optimise.

If we want to apply for an optmised and bounded search in the hyper-parameter space, I strongly suggest to take a look at:

- `Keras + hyperopt == hyperas`: http://maxpumperla.github.io/hyperas/