Assignment 04. Basics of neural networks final

October 9, 2019

1 Assignment for practical work 4. Basics of neural networks

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1.0.1 Using dataset: Page Blocks Dataset

Page Blocks Dataset

1.1 General Assignment

Before performing the practical work, you need download the data set accordingly to the option on your machine 1. Write a program that splits the original sample into a training set and a test set (training set, validation set, test set) 2. Build a model using Perceptron (http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Perceptron.html) and MLPClassifier (http://scikit-learn.org/stable/modules/generated/sklearn.neural_network.MLPClassifier.html). On the basis of experiments, select values for learning rate, the regularization parameter, the optimization function. 3. Build learning curves for better explanation of your experiments.

1.2 Options

Data sets are taken from the UCI Machine Learning Repository https://archive.ics.uci.edu/ml/ The option is determined by the data set, which can be downloaded from the link above: The option is determined by the data set, which can be downloaded from the link above: 1. Sponge 2. Water Treatment Plant 3. Synthetic Control Chart Time Series 4. Character Trajectories 5. Plants 6. Libras Movement 7. KEGG Metabolic Relation Network (Directed) 8. SMS Spam Collection 9. seeds 10. Human Activity Recognition Using Smartphones 11. User Knowledge Modeling 12. NYSK 13. Activities of Daily Living (ADLs) Recognition Using Binary Sensors 14. Dresses_Attribute_Sales 15. Wholesale customers 16. StoneFlakes 17. Gesture Phase Segmentation 18. AAAI 2014 Accepted Papers 19. Dow Jones Index 20. AAAI 2013 Accepted Papers 21. wiki4HE 22. Folio 23. Mice Protein Expression 24. Improved Spiral Test Using Digitized Graphics Tablet for Monitoring Parkinson's Disease

[1]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
```

```python
from sklearn.model_selection import train_test_split, cross_val_predict,␣
↪cross_val_score, GridSearchCV, RandomizedSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.impute import SimpleImputer
from sklearn.pipeline import Pipeline, make_pipeline
from sklearn.compose import ColumnTransformer
from sklearn.feature_selection import SelectFromModel
from sklearn.neural_network import MLPClassifier
from sklearn.linear_model import Perceptron
from sklearn.metrics import accuracy_score, classification_report
from sklearn.model_selection import validation_curve, learning_curve
from sklearn.preprocessing import LabelEncoder
from sklearn.preprocessing import OrdinalEncoder
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from keras import models
from keras import layers
from keras import utils
from keras import optimizers
```

```
Using TensorFlow backend.
```

[2]:
```python
def plot_learning_curve(estimator, title, X, y, ylim=None, cv=None,
                        n_jobs=None, train_sizes=np.linspace(.1, 1.0, 5)):
    plt.figure(figsize=(9,9))
    plt.title(title)
    if ylim is not None:
        plt.ylim(*ylim)
    plt.xlabel("Training examples")
    plt.ylabel("Score")
    train_sizes, train_scores, test_scores = learning_curve(
        estimator, X, y, cv=cv, n_jobs=n_jobs, train_sizes=train_sizes)
    train_scores_mean = np.mean(train_scores, axis=1)
    train_scores_std = np.std(train_scores, axis=1)
    test_scores_mean = np.mean(test_scores, axis=1)
    test_scores_std = np.std(test_scores, axis=1)
    plt.grid()

    plt.fill_between(train_sizes, train_scores_mean - train_scores_std,
                     train_scores_mean + train_scores_std, alpha=0.1,
                     color="orange")
    plt.fill_between(train_sizes, test_scores_mean - test_scores_std,
                     test_scores_mean + test_scores_std, alpha=0.1)
    plt.plot(train_sizes, train_scores_mean, 'o-', color="darkorange",
             label="Training score")
    plt.plot(train_sizes, test_scores_mean, 'o-',
             label="Cross-validation score")
```

```
    plt.legend(loc="best")
    return plt
```

[3]:
```
def plot_validation_curve(estimator, title, X, y, param_name, param_range,␣
 ↪scoring="accuracy"):
    train_scores, test_scores = validation_curve(
        estimator, X, y, param_name=param_name, param_range=param_range,
        cv=3, scoring=scoring, n_jobs=-1)
    train_scores_mean = np.mean(train_scores, axis=1)
    train_scores_std = np.std(train_scores, axis=1)
    test_scores_mean = np.mean(test_scores, axis=1)
    test_scores_std = np.std(test_scores, axis=1)


    best_test_param = param_range[np.argmax(test_scores_mean)]
    best_train_param = param_range[np.argmax(train_scores_mean)]

    best_test_score = np.max(test_scores_mean)
    best_train_score = np.max(train_scores_mean)


    plt.figure(figsize=(9,9))
    plt.title("Validation Curve {}: {} vs {}\nBest train param: {} - score:␣
 ↪{}\nBest test param: {} - score {}".format(title,
                                                                                ␣
 ↪                                    scoring,
                                                                                ␣
 ↪                                    param_name,
                                                                                ␣
 ↪                                    best_train_param,
                                                                                ␣
 ↪                                    best_train_score,
                                                                                ␣
 ↪                                    best_test_param,
                                                                                ␣
 ↪                                    best_test_score))
    plt.xlabel("{}".format(param_name))
    plt.ylabel("{}".format(scoring))
    #plt.ylim(0.1, 0.4)
    plt.axvline(best_test_param, color='darkorange', linestyle='--', label="best␣
 ↪train param")
    plt.axvline(best_train_param, color='navy', linestyle='--', label="best test␣
 ↪param")
    lw = 2
    plt.semilogx(param_range, train_scores_mean, label="Training score",
                 color="darkorange", lw=lw)
```

```
    plt.fill_between(param_range, train_scores_mean - train_scores_std,
                     train_scores_mean + train_scores_std, alpha=0.2,
                     color="darkorange", lw=lw)
    plt.semilogx(param_range, test_scores_mean, label="Cross-validation score",␣
↪lw=lw)
    plt.fill_between(param_range, test_scores_mean - test_scores_std,
                     test_scores_mean + test_scores_std, alpha=0.2, lw=lw)
    plt.legend(loc="best")
    plt.show()
```

2 Page-Blocks dataset

[4]:
```
elements = []
with open('data/page-blocks.data') as f:
    for l in f:
        elements.append([float(x) for x in l.split()])

elements = np.array(elements)
```

[5]:
```
columns = ['height',
           'lenght',
           'area',
           'eccen',
           'p_black',
           'p_and',
           'mean_tr',
           'blackpix',
           'blackand',
           'wb_trans',
           'block']
```

[6]:
```
df = pd.DataFrame(elements, columns=columns)
```

[7]:
```
X_train, X_test, y_train, y_test = train_test_split(df.drop("block", axis=1),␣
↪df["block"], train_size=0.7, random_state=42)
```

[8]:
```
X_train.describe()
```

[8]:
```
            height       lenght           area        eccen      p_black  \
count  3831.000000  3831.000000    3831.000000  3831.000000  3831.000000
mean     10.168102    88.115636    1182.607935    13.197051     0.367214
std      14.038977   114.094530    4999.354600    29.384528     0.176054
min       1.000000     1.000000       7.000000     0.007000     0.052000
25%       7.000000    17.000000     112.000000     2.111000     0.261000
50%       8.000000    40.000000     320.000000     5.111000     0.337000
75%      10.000000   104.000000     960.000000    13.309500     0.424000
max     311.000000   553.000000  143993.000000   413.000000     1.000000
```

```
            p_and      mean_tr      blackpix      blackand      wb_trans
count  3831.000000  3831.000000   3831.000000   3831.000000  3831.000000
mean      0.785362     6.415409    354.974158    725.282172   105.078831
std       0.170014    81.630229   1302.946891   1912.952788   162.250784
min       0.062000     1.000000      7.000000      7.000000     1.000000
25%       0.680500     1.610000     42.000000     94.000000    17.000000
50%       0.804000     2.070000    105.000000    246.000000    48.000000
75%       0.925000     2.990000    278.000000    698.500000   123.000000
max       1.000000  4955.000000  33017.000000  46133.000000  3212.000000
```

2.1 Normalizing the data

[9]:
```
scale = StandardScaler()
```

[10]:
```
X_train_scaled = pd.DataFrame(scale.fit_transform(X_train), columns=X_train.
 ↪columns)
```

3 Perceptron

3.1 Comparing performance of scaled and unscaled data

Unscaled inputs

[11]:
```
cv_scores = cross_val_score(Perceptron(random_state=42), X_train, y_train, cv=5,␣
 ↪n_jobs=-1, scoring="accuracy")
cv_scores
```

[11]:
```
array([0.93237971, 0.73307292, 0.67232376, 0.91361257, 0.93193717])
```

[12]:
```
np.mean(cv_scores)
```

[12]:
```
0.836665225718372
```

Scaled inputs

[13]:
```
cv_scores = cross_val_score(Perceptron(random_state=42), X_train_scaled,␣
 ↪y_train, cv=5, n_jobs=-1, scoring="accuracy")
cv_scores
```

[13]:
```
array([0.90117035, 0.94270833, 0.96605744, 0.95287958, 0.94240838])
```

[14]:
```
np.mean(cv_scores)
```

[14]:
```
0.9410448167614224
```

The (unoptimized) model performs much better with the scaled inputs. We will therefore use the scaled inputs for further analysis.

3.2 Tuning hyperparameters

As we've seen above the cross-validation accuracy of both models is already pretty high (94%-97%). Let's see how much we can improve the models by tuning hyperparameters.

[15]:
```
param_perc_dist = {"penalty":[None, 'l1', 'l2', 'elasticnet'],
                   "alpha":np.logspace(-7, 0, 30),
                   "max_iter" : np.arange(100,2000, 200),
                   "eta0": [0.1, 0.5, 1]}
```

[16]:
```
rand_perc = RandomizedSearchCV(Perceptron(random_state=42),␣
 ↪param_distributions=param_perc_dist, n_iter=500, scoring="accuracy", cv=3,␣
 ↪verbose=1, random_state=42)
```

[17]:
```
rand_perc.fit(X_train_scaled, y_train)
```

```
Fitting 3 folds for each of 500 candidates, totalling 1500 fits

[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.
[Parallel(n_jobs=1)]: Done 1500 out of 1500 | elapsed:   16.3s finished
```

[17]:
```
RandomizedSearchCV(cv=3, error_score='raise-deprecating',
                   estimator=Perceptron(alpha=0.0001, class_weight=None,
                                        early_stopping=False, eta0=1.0,
                                        fit_intercept=True, max_iter=1000,
                                        n_iter_no_change=5, n_jobs=None,
                                        penalty=None, random_state=42,
                                        shuffle=True, tol=0.001,
                                        validation_fraction=0.1, verbose=0,
                                        warm_start=False),
                   iid='warn', n_iter=500, n_jobs=None,
                   param_dist...
       6.72335754e-03, 1.17210230e-02, 2.04335972e-02, 3.56224789e-02,
       6.21016942e-02, 1.08263673e-01, 1.88739182e-01, 3.29034456e-01,
       5.73615251e-01, 1.00000000e+00]),
                                        'eta0': [0.1, 0.5, 1],
                                        'max_iter': array([ 100,  300,  500,
700,  900, 1100, 1300, 1500, 1700, 1900]),
                                        'penalty': [None, 'l1', 'l2',
                                                    'elasticnet']},
                   pre_dispatch='2*n_jobs', random_state=42, refit=True,
                   return_train_score=False, scoring='accuracy', verbose=1)
```

[18]:
```
perc_best_penalty, perc_best_max_iter = rand_perc.best_params_['penalty'],␣
 ↪rand_perc.best_params_['max_iter']
```

[19]:
```
rand_perc.best_params_, rand_perc.best_score_
```

[19]:
```
({'penalty': 'l1',
  'max_iter': 1300,
  'eta0': 0.5,
```

```
 'alpha': 2.8072162039411756e-06},
 0.9556251631427826)
```

Out of those 2500 fits the 'l1' regularization and max_iter=1300 come out as most favourable. We will now look a bit closer at eta0, the learning rate, and alpha, the constant multiplying the regularization term.

[20]:
```python
param_perc_grid = {'alpha':np.logspace(-7,0, 50),
                   'eta0':np.logspace(-4,0, 30)}
grid_perc = GridSearchCV(Perceptron(penalty=perc_best_penalty,␣
 ↪max_iter=perc_best_max_iter, random_state=42), param_grid=param_perc_grid,␣
 ↪scoring="accuracy", n_jobs=-1, cv=5)
```

[21]:
```python
grid_perc.fit(X_train_scaled, y_train)
```

```
/home/snbl/HDD/anaconda3/lib/python3.7/site-
packages/sklearn/model_selection/_search.py:813: DeprecationWarning: The default
of the `iid` parameter will change from True to False in version 0.22 and will
be removed in 0.24. This will change numeric results when test-set sizes are
unequal.
  DeprecationWarning)
```

[21]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
             estimator=Perceptron(alpha=0.0001, class_weight=None,
                                  early_stopping=False, eta0=1.0,
                                  fit_intercept=True, max_iter=1300,
                                  n_iter_no_change=5, n_jobs=None, penalty='l1',
                                  random_state=42, shuffle=True, tol=0.001,
                                  validation_fraction=0.1, verbose=0,
                                  warm_start=False),
             iid='warn', n_jobs=-1,
             param_grid={'alpha': array([1...
       4.52035366e-03, 6.21016942e-03, 8.53167852e-03, 1.17210230e-02,
       1.61026203e-02, 2.21221629e-02, 3.03919538e-02, 4.17531894e-02,
       5.73615251e-02, 7.88046282e-02, 1.08263673e-01, 1.48735211e-01,
       2.04335972e-01, 2.80721620e-01, 3.85662042e-01, 5.29831691e-01,
       7.27895384e-01, 1.00000000e+00])},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

[22]:
```python
perc_best_alpha, perc_best_eta0 = grid_perc.best_params_['alpha'], grid_perc.
 ↪best_params_['eta0']
```

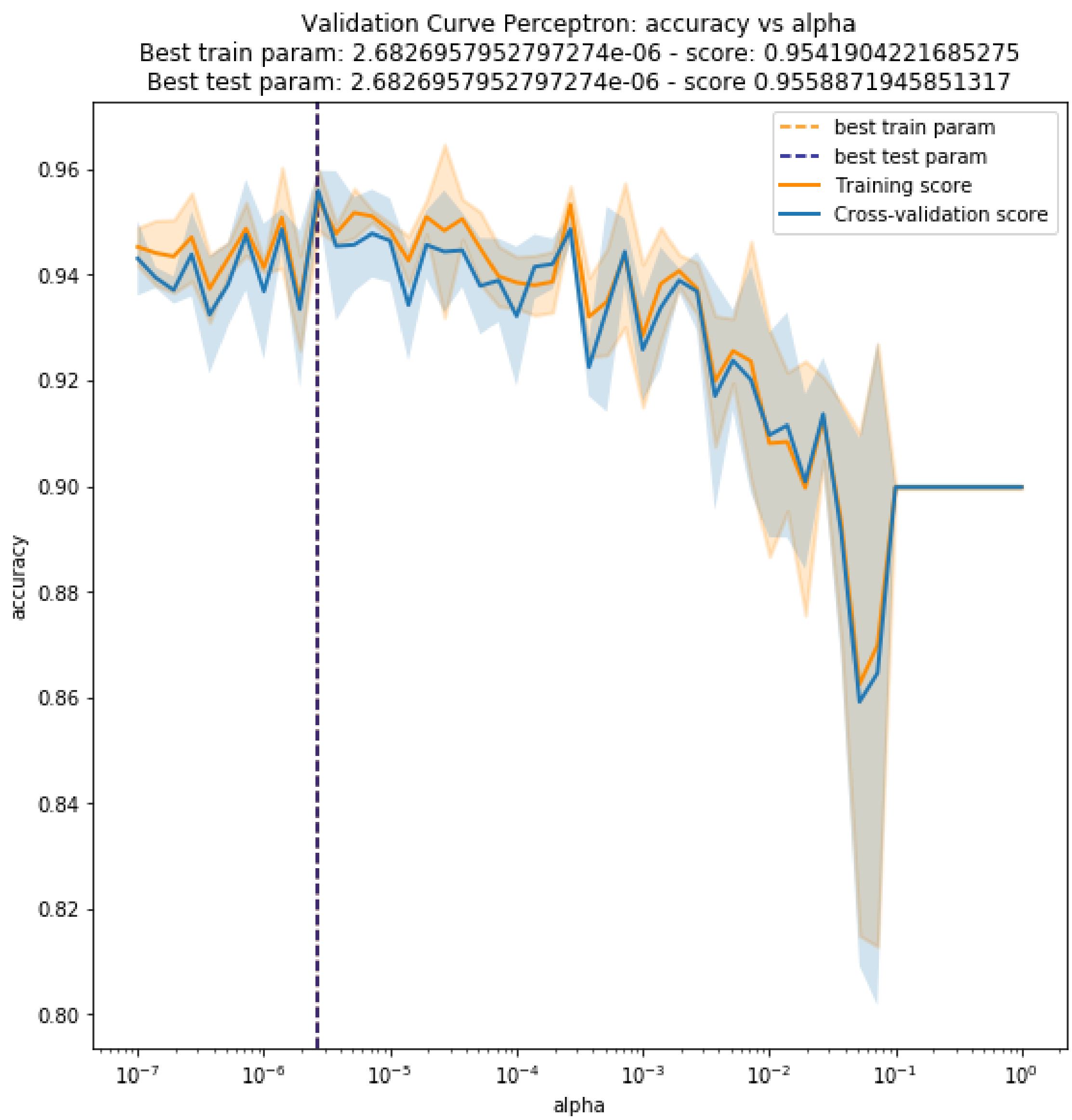
[23]:
```python
grid_perc.best_params_, grid_perc.best_score_
```

[23]:
```
({'alpha': 0.00019306977288832496, 'eta0': 0.1082636733874054},
 0.953275907073871)
```

3.3 Validation curves

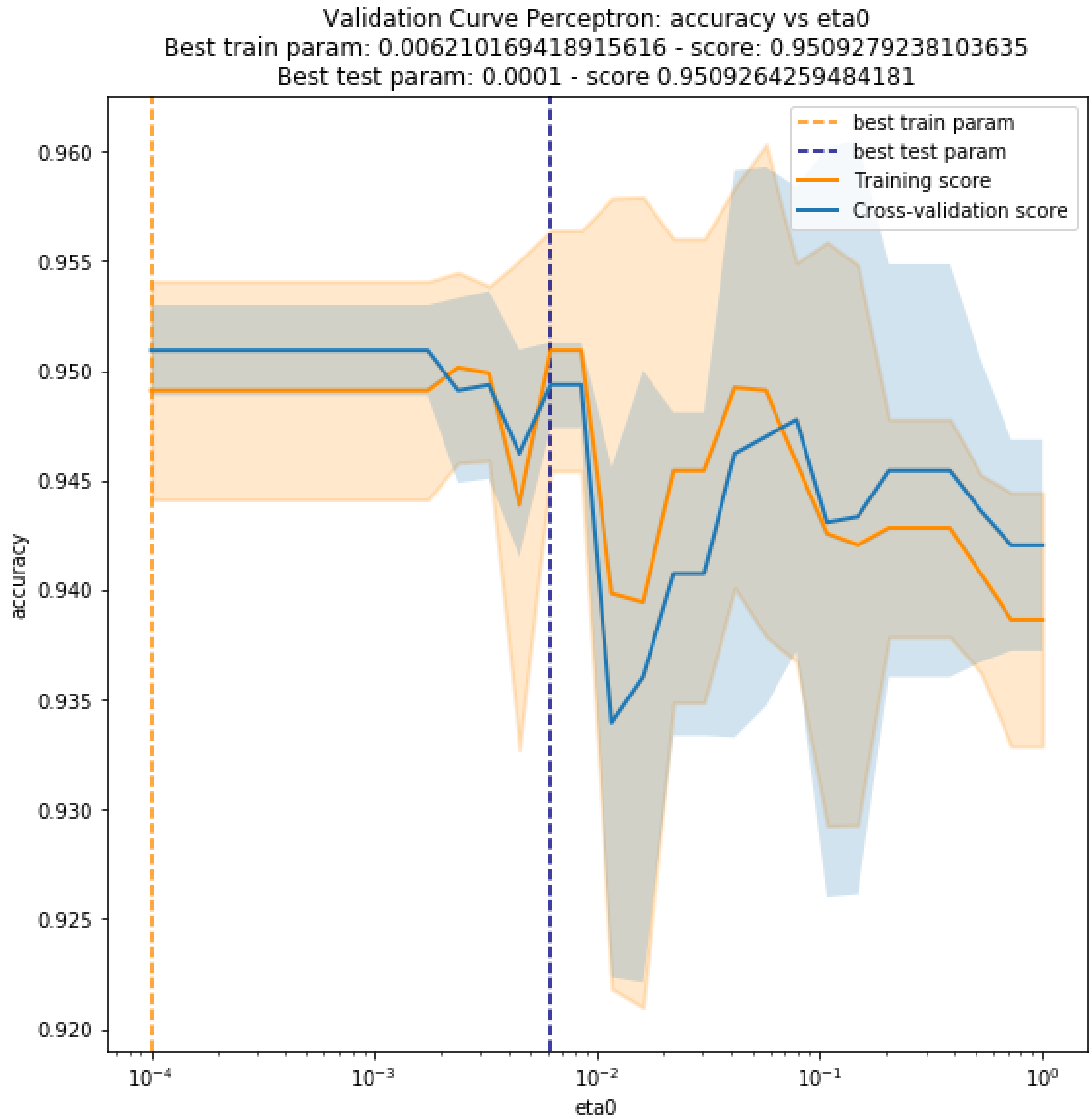
Performing an exhaustive grid search over eta0 and alpha lead to slightly different parameters and an increase in accuracy of 0.1%. Let's look at validation curves for both parameters independently.

[24]:
```
plot_validation_curve(Perceptron(penalty=perc_best_penalty,
                                 alpha=perc_best_eta0,
                                 max_iter=perc_best_max_iter,
                                 random_state=42), "Perceptron", X_train_scaled,␣
 ↪y_train, "alpha", param_perc_grid['alpha'])
```



[25]:
```
plot_validation_curve(Perceptron(penalty=perc_best_penalty,
                                 alpha=perc_best_alpha,
```

```
                                          max_iter=perc_best_max_iter,
                                          random_state=42), "Perceptron", X_train_scaled,␣
↪y_train, "eta0", param_perc_grid['eta0'])
```

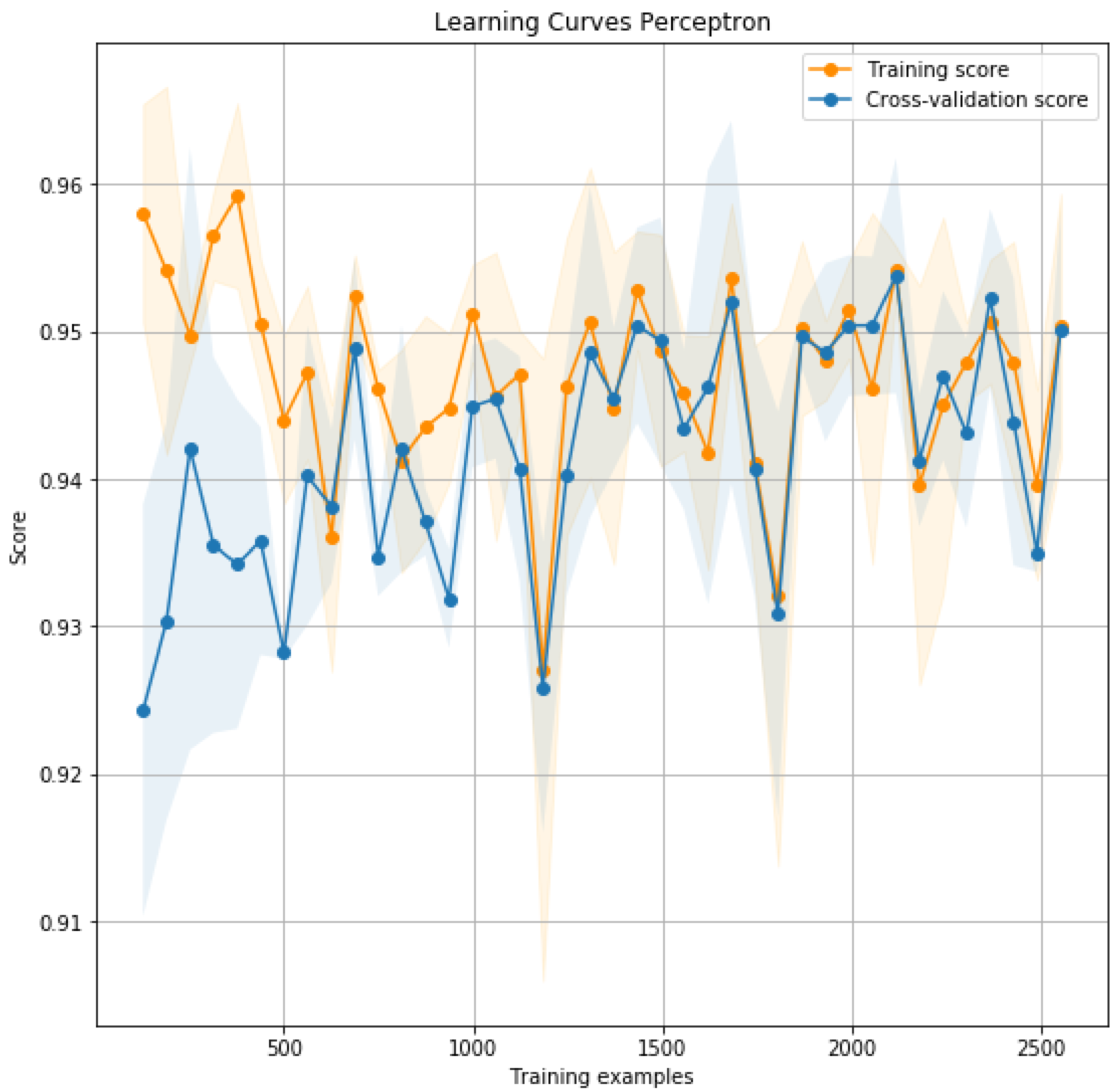


3.4 Learning curve

Let's take a look at the learning curve using the best parameters found through Randomized-SearchCV and GridSearchCV.

[26]:
```
perc = Perceptron(random_state=42,
                  penalty=perc_best_penalty,
                  alpha=perc_best_alpha,
                  eta0=perc_best_eta0,
```

```
                    max_iter=perc_best_max_iter)
plot_learning_curve(perc, "Learning Curves Perceptron", X_train_scaled, y_train,␣
 ↪cv=3, n_jobs=-1,
                      train_sizes=np.linspace(0.05,1, 40))

plt.show()
```



We can see the training and test score converge with 94%-95% accuracy. This means that our model is neither underfitted nor overfitted.

The best score we could reach through tuning with GridSearchCV was 95.3% accuracy, which is ~0.3% higher than the Perceptron model with default parameters.

4 Multi Layer Perceptron Classifier

Unscaled inputs

[27]:
```
cv_scores = cross_val_score(MLPClassifier(random_state=42), X_train, y_train,␣
↪cv=5, n_jobs=-1, scoring="accuracy")
cv_scores
```

[27]:
```
array([0.95968791, 0.96614583, 0.96475196, 0.88481675, 0.96073298])
```

[28]:
```
np.mean(cv_scores)
```

[28]:
```
0.9472270872299366
```

Scaled inputs

[29]:
```
cv_scores = cross_val_score(MLPClassifier(random_state=42), X_train_scaled,␣
↪y_train, cv=5, n_jobs=-1, scoring="accuracy")
cv_scores
```

[29]:
```
array([0.96358908, 0.96223958, 0.97911227, 0.98167539, 0.97120419])
```

[30]:
```
np.mean(cv_scores)
```

[30]:
```
0.9715641025497306
```

We find that the MLPClassifier like the Perceptron responds to the scaled data with increased accuracy.

4.1 Tuning hyperparameters

As we've seen above the cross-validation accuracy of the model is already pretty high (97.1%). Let's see how much we can improve the model by tuning hyperparameters. Before we start looking at the learning rate and regularization parameter, we will search for a good number of hidden layers and their respective sizes.

Find the optimal layer sizes

[31]:
```
param_mlp_grid = {'hidden_layer_sizes' : [(x,) for x in np.arange(100, 500,␣
↪100)] + [(x,y) for x in np.arange(100, 500, 100) for y in np.arange(100, 500,␣
↪200)],
                  'solver': ['lbfgs', 'sgd', 'adam'],
                  'learning_rate': ['constant', 'invscaling', 'adaptive']}
```

[32]:
```
grid_mlp = GridSearchCV(MLPClassifier(random_state=42),␣
↪param_grid=param_mlp_grid, scoring="accuracy", cv=3, n_jobs=-1, verbose=5)
grid_mlp.fit(X_train_scaled, y_train)
```

```
Fitting 3 folds for each of 108 candidates, totalling 324 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done   2 tasks      | elapsed:    6.5s
[Parallel(n_jobs=-1)]: Done  56 tasks      | elapsed:  2.8min
```

```
[Parallel(n_jobs=-1)]: Done 146 tasks      | elapsed: 15.1min
[Parallel(n_jobs=-1)]: Done 272 tasks      | elapsed: 44.3min
[Parallel(n_jobs=-1)]: Done 324 out of 324 | elapsed: 59.7min finished
```

[32]:
```
GridSearchCV(cv=3, error_score='raise-deprecating',
             estimator=MLPClassifier(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,),
                                     learning_rate='constant',
                                     learning_rate_init=0.001, max_iter=200,
                                     momentum=0.9, n_iter_no_change=10,
                                     nesterovs_momentum=True, power_t=0.5,
                                     random_sta...
                                     warm_start=False),
             iid='warn', n_jobs=-1,
             param_grid={'hidden_layer_sizes': [(100,), (200,), (300,), (400,),
                                                (100, 100), (100, 300),
                                                (200, 100), (200, 300),
                                                (300, 100), (300, 300),
                                                (400, 100), (400, 300)],
                         'learning_rate': ['constant', 'invscaling',
                                           'adaptive'],
                         'solver': ['lbfgs', 'sgd', 'adam']},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=5)
```

[33]:
```
mlp_best_hidden_layers, mlp_best_solver = grid_mlp.
 ↪best_params_['hidden_layer_sizes'], grid_mlp.best_params_['solver']
```

[34]:
```
grid_mlp.best_params_, grid_mlp.best_score_
```

[34]:
```
({'hidden_layer_sizes': (400,), 'learning_rate': 'constant', 'solver': 'adam'},
 0.9731140694335683)
```

Great, a model with 2 hidden layers with 200 and 300 neurons utilizing the ADAM-optimizer results in an accuracy of 97.31% which is 0.2% higher than the default.

4.1.1 Learning Rate

Let's also see if there is a preferable behaviour of the learning rate

[35]:
```
param_mlp_grid = {'learning_rate' : ["constant", "invscaling", "adaptive"]}
grid_mlp = GridSearchCV(MLPClassifier(hidden_layer_sizes=mlp_best_hidden_layers,
                                      solver=mlp_best_solver,
                                      random_state=42,
                                      verbose=1),
                        param_grid=param_mlp_grid,
                        scoring="accuracy",
                        cv=3,
```

```
                         n_jobs=-1)
grid_mlp.fit(X_train_scaled, y_train)
```

```
Iteration 1, loss = 1.20594384
Iteration 2, loss = 0.58171118
Iteration 3, loss = 0.35838703
Iteration 4, loss = 0.27450555
Iteration 5, loss = 0.23271532
Iteration 6, loss = 0.20584371
Iteration 7, loss = 0.18803907
Iteration 8, loss = 0.17291697
Iteration 9, loss = 0.16176006
Iteration 10, loss = 0.15194128
Iteration 11, loss = 0.14458041
Iteration 12, loss = 0.13780352
Iteration 13, loss = 0.13345655
Iteration 14, loss = 0.12894605
Iteration 15, loss = 0.12430279
Iteration 16, loss = 0.12142584
Iteration 17, loss = 0.11782709
Iteration 18, loss = 0.11562424
Iteration 19, loss = 0.11238660
Iteration 20, loss = 0.11050041
Iteration 21, loss = 0.10814165
Iteration 22, loss = 0.10732295
Iteration 23, loss = 0.10456546
Iteration 24, loss = 0.10339190
Iteration 25, loss = 0.10137862
Iteration 26, loss = 0.10012281
Iteration 27, loss = 0.09975509
Iteration 28, loss = 0.09874356
Iteration 29, loss = 0.09873309
Iteration 30, loss = 0.09607850
Iteration 31, loss = 0.09513540
Iteration 32, loss = 0.09442852
Iteration 33, loss = 0.09306321
Iteration 34, loss = 0.09262586
Iteration 35, loss = 0.09198412
Iteration 36, loss = 0.09072855
Iteration 37, loss = 0.09059752
Iteration 38, loss = 0.09050810
Iteration 39, loss = 0.08878780
Iteration 40, loss = 0.08930607
Iteration 41, loss = 0.08822544
Iteration 42, loss = 0.08737848
Iteration 43, loss = 0.08712787
Iteration 44, loss = 0.08736452
```

```
Iteration 45, loss = 0.08590706
Iteration 46, loss = 0.08605058
Iteration 47, loss = 0.08454668
Iteration 48, loss = 0.08553275
Iteration 49, loss = 0.08521164
Iteration 50, loss = 0.08431344
Iteration 51, loss = 0.08405978
Iteration 52, loss = 0.08293321
Iteration 53, loss = 0.08268093
Iteration 54, loss = 0.08390859
Iteration 55, loss = 0.08197434
Iteration 56, loss = 0.08105605
Iteration 57, loss = 0.08223233
Iteration 58, loss = 0.08027447
Iteration 59, loss = 0.08174414
Iteration 60, loss = 0.08119426
Iteration 61, loss = 0.08075425
Iteration 62, loss = 0.07849970
Iteration 63, loss = 0.07930598
Iteration 64, loss = 0.07893672
Iteration 65, loss = 0.07830536
Iteration 66, loss = 0.07818686
Iteration 67, loss = 0.07887624
Iteration 68, loss = 0.07814601
Iteration 69, loss = 0.07642535
Iteration 70, loss = 0.07601650
Iteration 71, loss = 0.07649912
Iteration 72, loss = 0.07628444
Iteration 73, loss = 0.07659082
Iteration 74, loss = 0.07601252
Iteration 75, loss = 0.07596417
Iteration 76, loss = 0.07975773
Iteration 77, loss = 0.07973533
Iteration 78, loss = 0.07570438
Iteration 79, loss = 0.07496322
Iteration 80, loss = 0.07410192
Iteration 81, loss = 0.07294308
Iteration 82, loss = 0.07342216
Iteration 83, loss = 0.07263076
Iteration 84, loss = 0.07349731
Iteration 85, loss = 0.07531825
Iteration 86, loss = 0.07263606
Iteration 87, loss = 0.07197627
Iteration 88, loss = 0.07194503
Iteration 89, loss = 0.07151808
Iteration 90, loss = 0.07105448
Iteration 91, loss = 0.07358689
Iteration 92, loss = 0.07103551
```

```
Iteration 93, loss = 0.07143558
Iteration 94, loss = 0.07120123
Iteration 95, loss = 0.07123164
Iteration 96, loss = 0.07005990
Iteration 97, loss = 0.07005678
Iteration 98, loss = 0.07026674
Iteration 99, loss = 0.07013851
Iteration 100, loss = 0.06976227
Iteration 101, loss = 0.07036089
Iteration 102, loss = 0.06850491
Iteration 103, loss = 0.06892461
Iteration 104, loss = 0.06878299
Iteration 105, loss = 0.06917141
Iteration 106, loss = 0.06885433
Iteration 107, loss = 0.06976566
Iteration 108, loss = 0.06874874
Iteration 109, loss = 0.06787731
Iteration 110, loss = 0.06799667
Iteration 111, loss = 0.06778775
Iteration 112, loss = 0.06741751
Iteration 113, loss = 0.06787096
Iteration 114, loss = 0.06927643
Iteration 115, loss = 0.06793906
Iteration 116, loss = 0.06680089
Iteration 117, loss = 0.06818715
Iteration 118, loss = 0.06641362
Iteration 119, loss = 0.06740877
Iteration 120, loss = 0.06594947
Iteration 121, loss = 0.06578001
Iteration 122, loss = 0.06712512
Iteration 123, loss = 0.06721550
Iteration 124, loss = 0.06862681
Iteration 125, loss = 0.06579735
Iteration 126, loss = 0.06513458
Iteration 127, loss = 0.06525450
Iteration 128, loss = 0.06639043
Iteration 129, loss = 0.06546997
Iteration 130, loss = 0.06408660
Iteration 131, loss = 0.06700166
Iteration 132, loss = 0.06448245
Iteration 133, loss = 0.06530527
Iteration 134, loss = 0.06525875
Iteration 135, loss = 0.06569526
Iteration 136, loss = 0.06567089
Iteration 137, loss = 0.06462872
Iteration 138, loss = 0.06371865
Iteration 139, loss = 0.06575052
Iteration 140, loss = 0.06522836
```

```
Iteration 141, loss = 0.06345325
Iteration 142, loss = 0.06483320
Iteration 143, loss = 0.06374680
Iteration 144, loss = 0.06379601
Iteration 145, loss = 0.06429549
Iteration 146, loss = 0.06391749
Iteration 147, loss = 0.06377973
Iteration 148, loss = 0.06316592
Iteration 149, loss = 0.06226852
Iteration 150, loss = 0.06177262
Iteration 151, loss = 0.06240937
Iteration 152, loss = 0.06247667
Iteration 153, loss = 0.06279214
Iteration 154, loss = 0.06215455
Iteration 155, loss = 0.06259976
Iteration 156, loss = 0.06326125
Iteration 157, loss = 0.06142294
Iteration 158, loss = 0.06237537
Iteration 159, loss = 0.06258681
Iteration 160, loss = 0.06140277
Iteration 161, loss = 0.06202721
Iteration 162, loss = 0.06342611
Iteration 163, loss = 0.06659235
Iteration 164, loss = 0.06222654
Iteration 165, loss = 0.06145126
Iteration 166, loss = 0.06175951
Iteration 167, loss = 0.06011054
Iteration 168, loss = 0.06108162
Iteration 169, loss = 0.06024880
Iteration 170, loss = 0.06220417
Iteration 171, loss = 0.06108180
Iteration 172, loss = 0.06034935
Iteration 173, loss = 0.06207455
Iteration 174, loss = 0.06041303
Iteration 175, loss = 0.06287171
Iteration 176, loss = 0.06031411
Iteration 177, loss = 0.06100331
Iteration 178, loss = 0.06004364
Training loss did not improve more than tol=0.000100 for 10 consecutive epochs.
Stopping.
```

[35]:
```
GridSearchCV(cv=3, error_score='raise-deprecating',
             estimator=MLPClassifier(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=(400,),
                                     learning_rate='constant',
```

```
                                        learning_rate_init=0.001, max_iter=200,
                                        momentum=0.9, n_iter_no_change=10,
                                        nesterovs_momentum=True, power_t=0.5,
                                        random_state=42, shuffle=True,
                                        solver='adam', tol=0.0001,
                                        validation_fraction=0.1, verbose=1,
                                        warm_start=False),
                    iid='warn', n_jobs=-1,
                    param_grid={'learning_rate': ['constant', 'invscaling',
                                                  'adaptive']},
                    pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
                    scoring='accuracy', verbose=0)
```

[36]:
```
mlp_best_learning_rate = grid_mlp.best_params_['learning_rate']
```

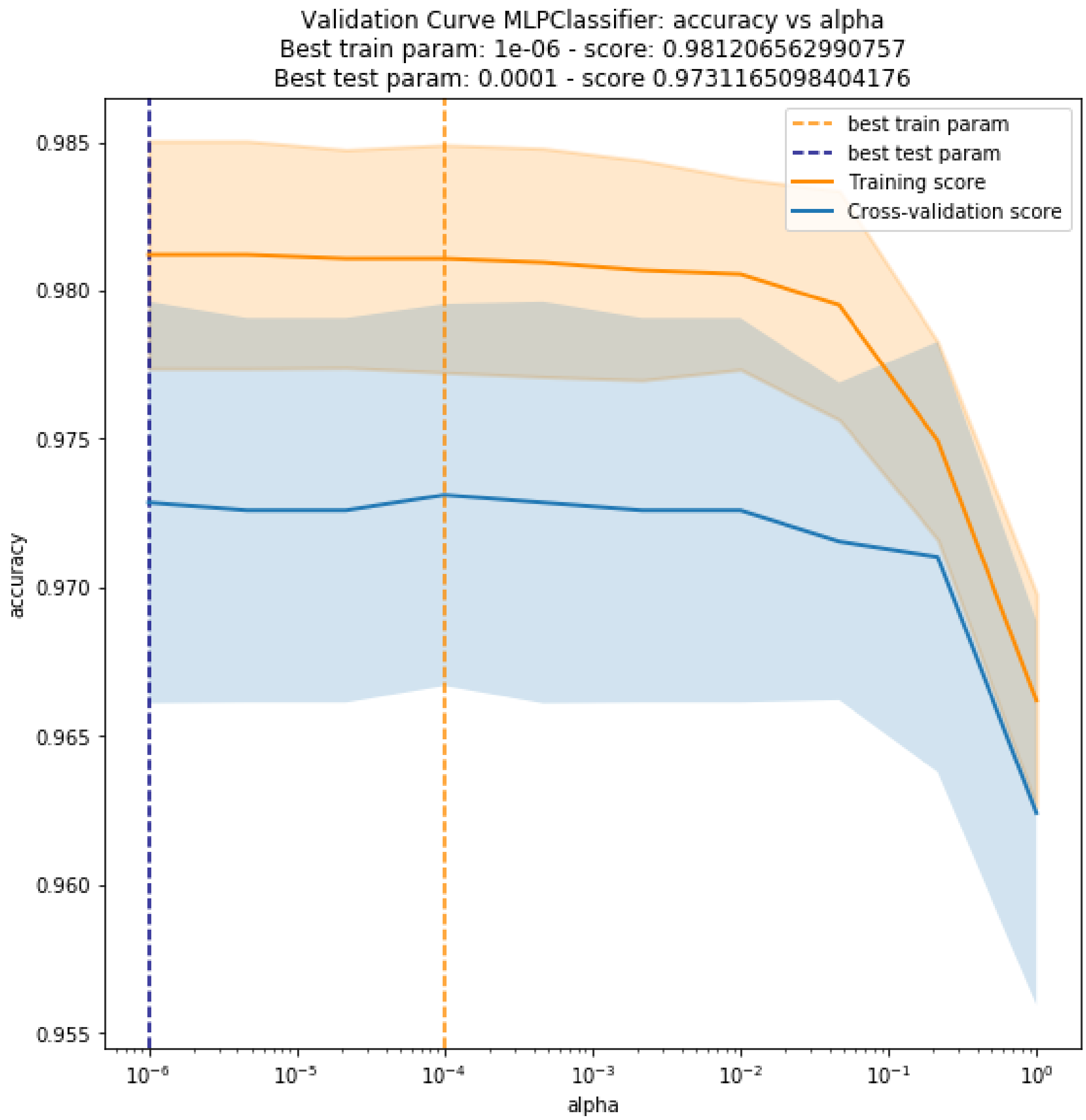
[37]:
```
grid_mlp.best_params_, grid_mlp.best_score_
```

[37]:
```
({'learning_rate': 'constant'}, 0.9731140694335683)
```

4.1.2 Find the optimal regularization parameter

Let us first look at a validation curve for the regularization parameter alpha

[38]:
```
param_mlp_grid = {'alpha' : np.logspace(-6,0, 10)}
plot_validation_curve(MLPClassifier(hidden_layer_sizes=mlp_best_hidden_layers,
                                    solver=mlp_best_solver,
                                    learning_rate=mlp_best_learning_rate,
                                    random_state=42), "MLPClassifier",␣
 ↪X_train_scaled, y_train, "alpha", param_mlp_grid['alpha'])
```



The training and cross-validation accuracy stays relatively the same over the full range of the alphas until both dramatically drop from 10^{-1} on.

[39]:
```
param_mlp_grid = {'alpha' : np.logspace(-6,-3, 4)}
grid_mlp = GridSearchCV(MLPClassifier(hidden_layer_sizes=mlp_best_hidden_layers,
                                       solver=mlp_best_solver,
                                       learning_rate=mlp_best_learning_rate,
                                       random_state=42),
                         param_grid=param_mlp_grid,
                         scoring="accuracy",
                         cv=3,
                         n_jobs=-1)
grid_mlp.fit(X_train_scaled, y_train)
```

[39]:
```
GridSearchCV(cv=3, error_score='raise-deprecating',
             estimator=MLPClassifier(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=(400,),
                                     learning_rate='constant',
                                     learning_rate_init=0.001, max_iter=200,
                                     momentum=0.9, n_iter_no_change=10,
                                     nesterovs_momentum=True, power_t=0.5,
                                     random_state=42, shuffle=True,
                                     solver='adam', tol=0.0001,
                                     validation_fraction=0.1, verbose=False,
                                     warm_start=False),
             iid='warn', n_jobs=-1,
             param_grid={'alpha': array([1.e-06, 1.e-05, 1.e-04, 1.e-03])},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

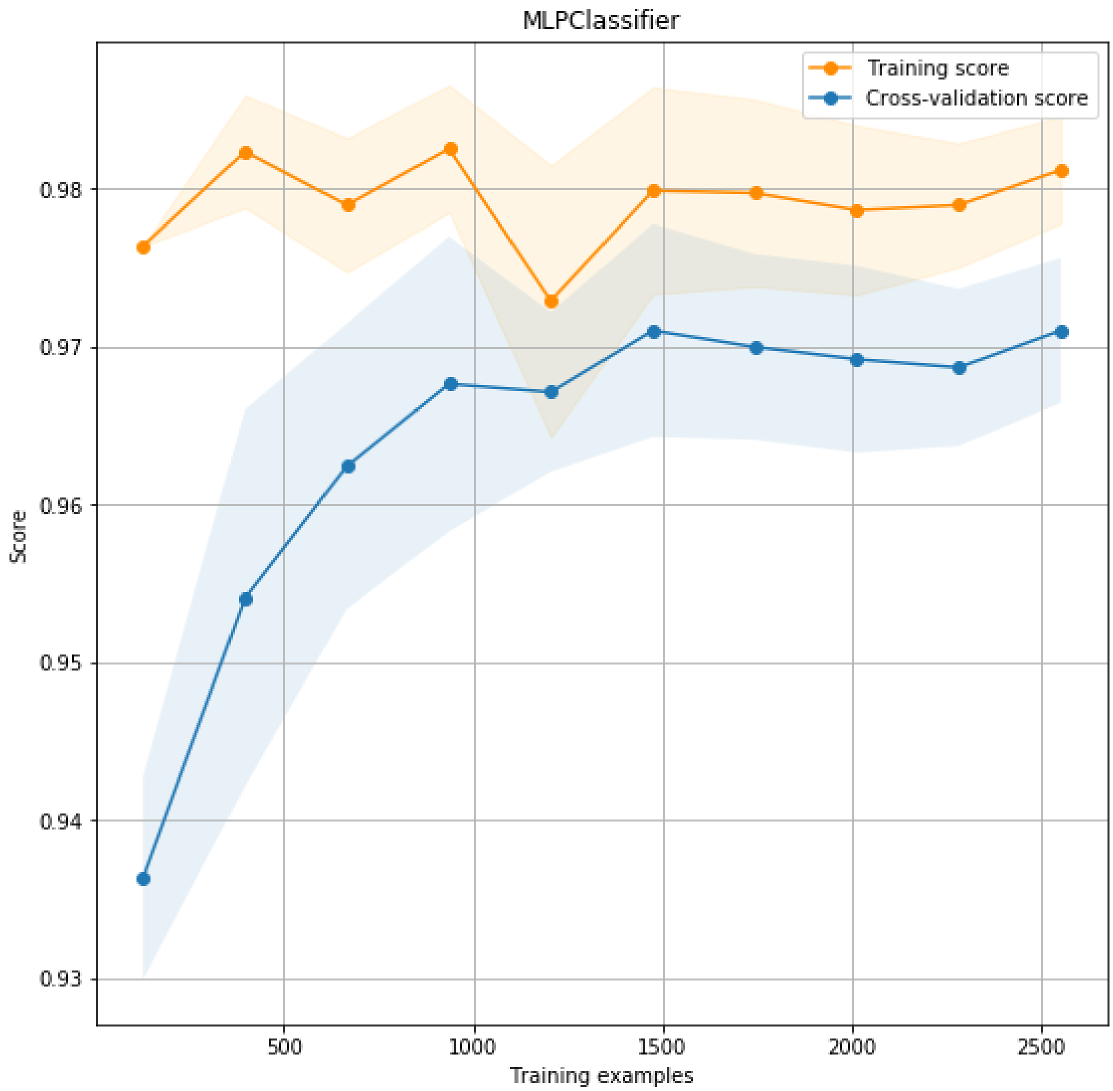
[40]:
```
mlp_best_alpha = grid_mlp.best_params_['alpha']
```

[41]:
```
grid_mlp.best_params_, grid_mlp.best_score_
```

[41]:
```
({'alpha': 0.0001}, 0.9731140694335683)
```

4.1.3 Learning curve

[42]:
```
mlp = MLPClassifier(hidden_layer_sizes=mlp_best_hidden_layers,
              learning_rate=mlp_best_learning_rate,
              solver=mlp_best_solver,
              alpha=mlp_best_alpha,
              random_state=42)

plot_learning_curve(mlp, "MLPClassifier", X_train_scaled, y_train, cv=3,␣
 ↪n_jobs=-1,
                    train_sizes=np.linspace(0.05, 1, 10))

plt.show()
```



We can see that the train and cross-validation scores initially being far apart converge to a difference of about 0.5%-1% accuracy.

5 Test scores

[43]:
```
X_test_scaled = scale.fit_transform(X_test)
```

5.0.1 Perceptron

[44]:
```
perc.fit(X_train_scaled, y_train)
perc_pred = perc.predict(X_test_scaled)
accuracy_score(y_test, perc_pred)
```

[44]: 0.9390986601705238

[45]:
```
print(classification_report(y_test, perc_pred))
```

```
              precision    recall  f1-score   support

         1.0       0.95      0.99      0.97      1466
         2.0       0.88      0.63      0.74       106
         3.0       0.50      0.70      0.58        10
         4.0       0.83      0.32      0.47        31
         5.0       0.71      0.34      0.47        29

    accuracy                           0.94      1642
   macro avg       0.78      0.60      0.64      1642
weighted avg       0.94      0.94      0.93      1642
```

5.0.2 Multi Layer Perceptron

[46]:
```
mlp.fit(X_train_scaled, y_train)
mlp_pred = mlp.predict(X_test_scaled)
accuracy_score(y_test, mlp_pred)
```

[46]: 0.9531059683313033

[47]:
```
print(classification_report(y_test, mlp_pred))
```

```
              precision    recall  f1-score   support

         1.0       0.96      0.99      0.98      1466
         2.0       0.89      0.75      0.82       106
         3.0       0.75      0.30      0.43        10
         4.0       0.89      0.55      0.68        31
         5.0       0.83      0.34      0.49        29

    accuracy                           0.95      1642
   macro avg       0.87      0.59      0.68      1642
weighted avg       0.95      0.95      0.95      1642
```

5.0.3 Random Forest and Gradient Boosting

Tuning the hyperparameters and fitting the models took a while. Let's s compare the results of the neural networks with a random forest and the gradient boosting algorithm.

[48]:
```
rf = RandomForestClassifier(n_estimators=200, random_state=42, n_jobs=-1)
cross_val_score(rf, X_train_scaled, y_train, scoring="accuracy", cv=10,␣
 ↪verbose=1)
```

```
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.
[Parallel(n_jobs=1)]: Done  10 out of  10 | elapsed:    6.7s finished
```

[48]:
```
array([0.96623377, 0.97142857, 0.95844156, 0.97135417, 0.96354167,
       0.984375  , 0.98694517, 0.97375328, 0.97368421, 0.97631579])
```

[49]:
```python
rf.fit(X_train_scaled, y_train)
```

[49]:
```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                       max_depth=None, max_features='auto', max_leaf_nodes=None,
                       min_impurity_decrease=0.0, min_impurity_split=None,
                       min_samples_leaf=1, min_samples_split=2,
                       min_weight_fraction_leaf=0.0, n_estimators=200,
                       n_jobs=-1, oob_score=False, random_state=42, verbose=0,
                       warm_start=False)
```

[50]:
```python
rf_pred = rf.predict(X_test_scaled)
accuracy_score(y_test, rf_pred)
```

[50]:
```
0.9579780755176613
```

[51]:
```python
print(classification_report(y_test, rf_pred))
```

```
              precision    recall  f1-score   support

         1.0       0.96      0.99      0.98      1466
         2.0       0.94      0.71      0.81       106
         3.0       0.62      0.50      0.56        10
         4.0       0.84      0.84      0.84        31
         5.0       0.85      0.38      0.52        29

    accuracy                           0.96      1642
   macro avg       0.84      0.68      0.74      1642
weighted avg       0.96      0.96      0.95      1642
```

5.0.4 XGBoost

[52]:
```python
xgb = GradientBoostingClassifier(n_estimators=100, max_features=5)
cross_val_score(xgb, X_train_scaled, y_train, scoring="accuracy", cv=10,␣
 ↪verbose=1)
```

```
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.
[Parallel(n_jobs=1)]: Done  10 out of  10 | elapsed:    9.8s finished
```

[52]:
```
array([0.96883117, 0.97662338, 0.96103896, 0.95833333, 0.96614583,
       0.97916667, 0.9843342 , 0.97112861, 0.96578947, 0.97894737])
```

[53]:
```python
xgb.fit(X_train_scaled, y_train)
xgb_pred = xgb.predict(X_test_scaled)
```

```
accuracy_score(y_test, xgb_pred)
```

[53]: 0.9549330085261876

[54]:
```
print(classification_report(y_test, xgb_pred))
```

```
              precision    recall  f1-score   support

         1.0       0.96      0.99      0.98      1466
         2.0       0.96      0.64      0.77       106
         3.0       1.00      0.40      0.57        10
         4.0       0.84      0.87      0.86        31
         5.0       0.72      0.45      0.55        29

    accuracy                           0.95      1642
   macro avg       0.90      0.67      0.75      1642
weighted avg       0.95      0.95      0.95      1642
```

5.0.5 Building a Neural Net Classifier with Keras

[55]:
```
y_train_ohe = utils.np_utils.to_categorical(y_train)
y_test_ohe = utils.np_utils.to_categorical(y_test)
```

[56]:
```
model = models.Sequential()
```

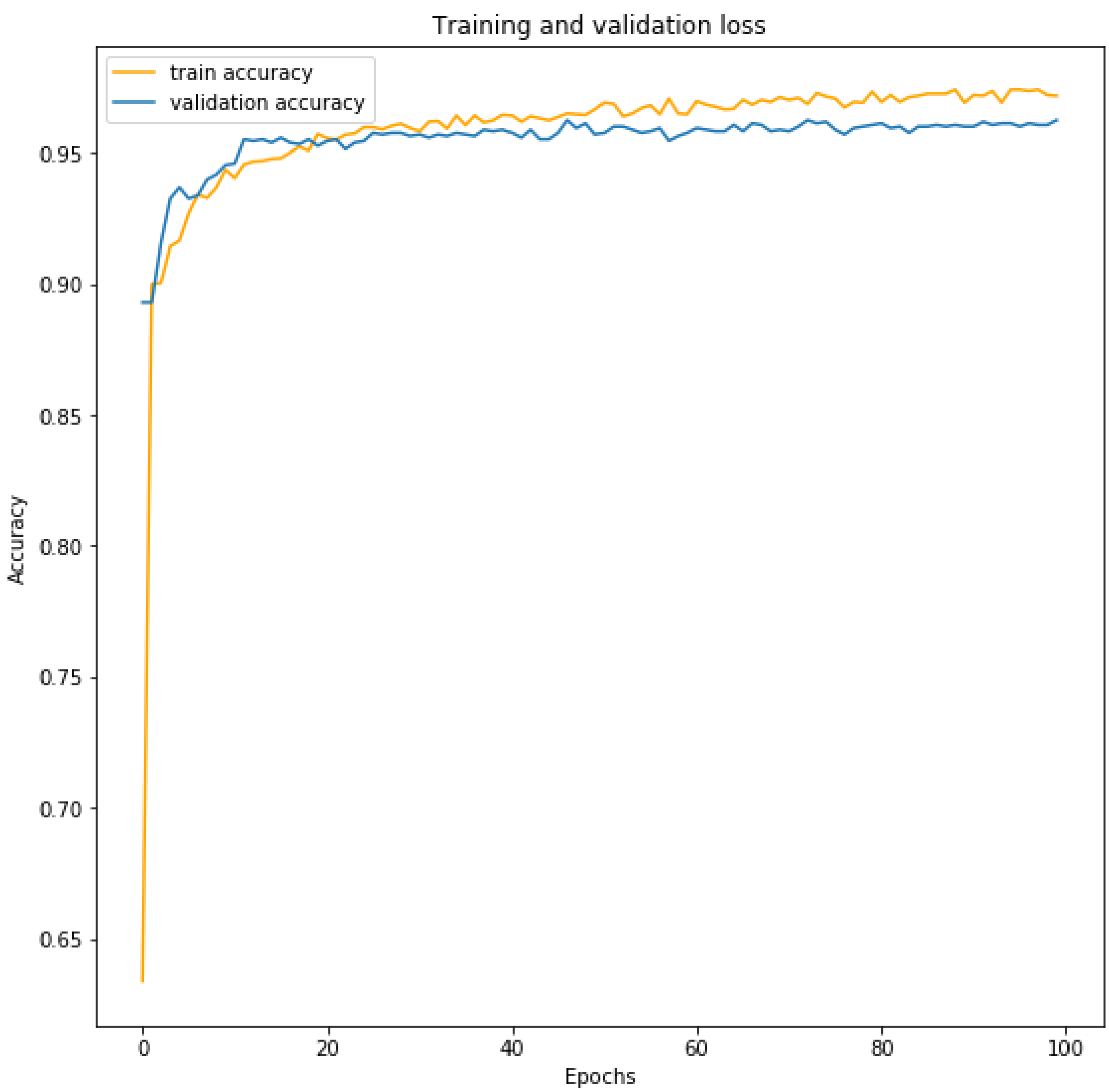
[57]:
```
model.add(layers.Dense(300, activation='relu', input_dim=10))
model.add(layers.Dropout(0.5))
model.add(layers.Dense(200, activation='relu'))
model.add(layers.Dropout(0.5))
model.add(layers.Dense(128, activation='tanh'))
model.add(layers.Dropout(0.4))
model.add(layers.Dense(64, activation='relu'))
model.add(layers.Dense(6, activation='softmax'))
```

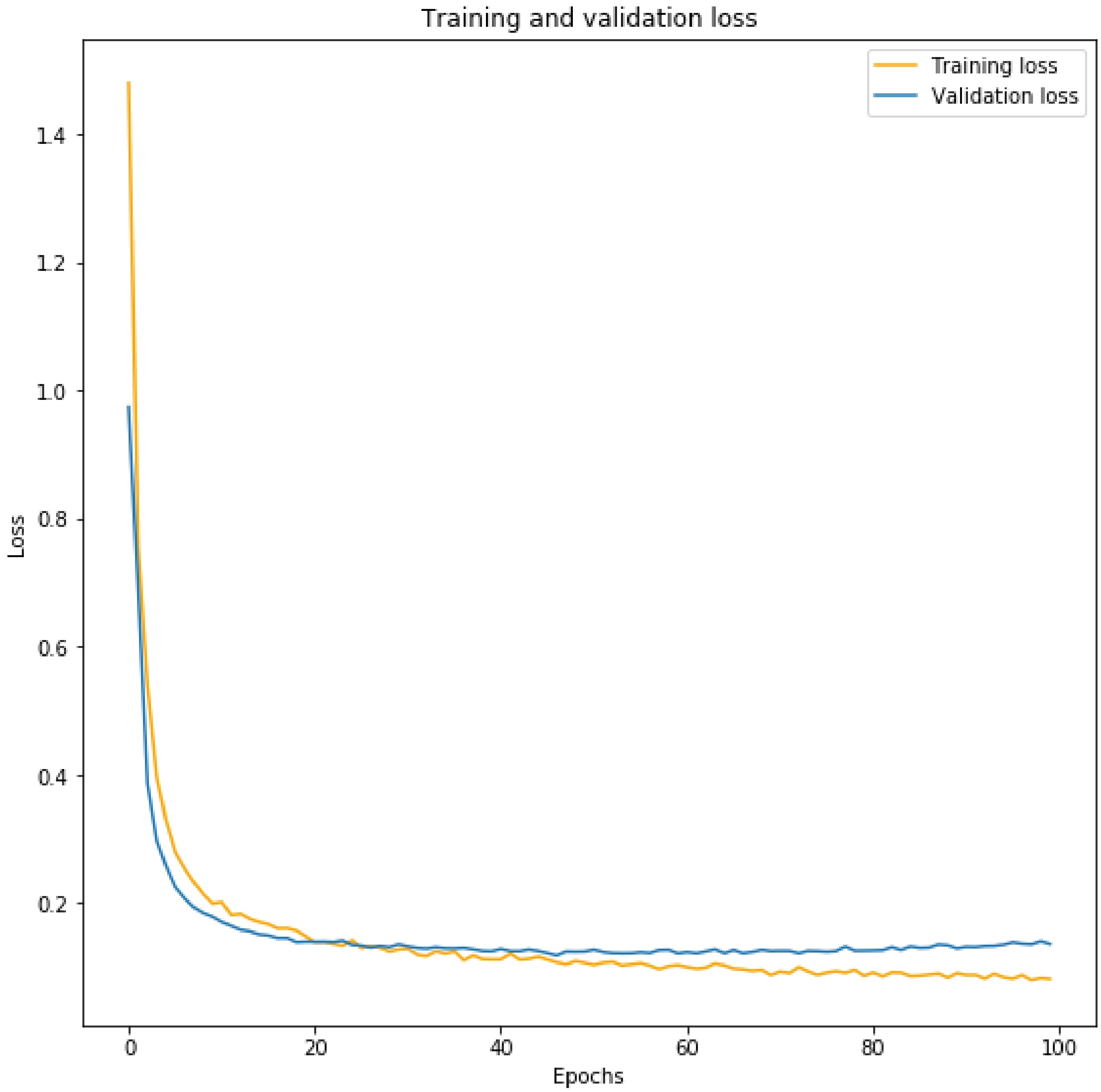
[58]:
```
model.compile(optimizer='adam',
              loss='categorical_crossentropy',
              metrics=['accuracy'])
```

[59]:
```
hist = model.fit(X_train_scaled,
                 y_train_ohe,
                 epochs=100,
                 workers=-1,
                 batch_size=512,
                 verbose=False,
                 validation_data=(X_test_scaled, y_test_ohe))
```

[60]:
```
plt.figure(figsize=(9,9))
plt.title('Training and validation loss')
```

```
plt.plot(hist.epoch, hist.history['accuracy'], color="orange", linestyle="-",␣
 ↪label="train accuracy")
plt.plot(hist.epoch, hist.history['val_accuracy'],  linestyle="-",␣
 ↪label="validation accuracy")
plt.ylabel("Accuracy")
plt.xlabel("Epochs")
plt.legend()


plt.figure(figsize=(9,9))
plt.plot(hist.epoch, hist.history['loss'], color="orange", label='Training loss')
plt.plot(hist.epoch, hist.history['val_loss'], label='Validation loss')
plt.ylabel("Loss")
plt.xlabel("Epochs")
plt.title('Training and validation loss')
plt.legend();
```





[61]:
```
pred_keras = model.predict_classes(X_test_scaled)
```

[62]:
```
print(classification_report(y_test, pred_keras))
```

```
              precision    recall  f1-score   support

         1.0       0.97      0.99      0.98      1466
         2.0       0.89      0.84      0.86       106
         3.0       0.71      0.50      0.59        10
         4.0       0.88      0.68      0.76        31
         5.0       0.76      0.45      0.57        29
```

```
    accuracy                           0.96      1642
   macro avg       0.84      0.69      0.75      1642
weighted avg       0.96      0.96      0.96      1642
```

Compared with the SciKit MLPClassifier

[63]:
```
print(classification_report(y_test, mlp_pred))
```

```
              precision    recall  f1-score   support

         1.0       0.96      0.99      0.98      1466
         2.0       0.89      0.75      0.82       106
         3.0       0.75      0.30      0.43        10
         4.0       0.89      0.55      0.68        31
         5.0       0.83      0.34      0.49        29

    accuracy                           0.95      1642
   macro avg       0.87      0.59      0.68      1642
weighted avg       0.95      0.95      0.95      1642
```

5.0.6 Convulutional Network

As a final experiment we tried fitting our data to a convolutional network.

[65]:
```
X_train_tensor = X_train_scaled.values.reshape(X_train_scaled.shape[0],␣
↪X_train_scaled.shape[1], 1)
X_test_tensor = X_test_scaled.reshape(X_test_scaled.shape[0], X_test_scaled.
↪shape[1], 1)
```

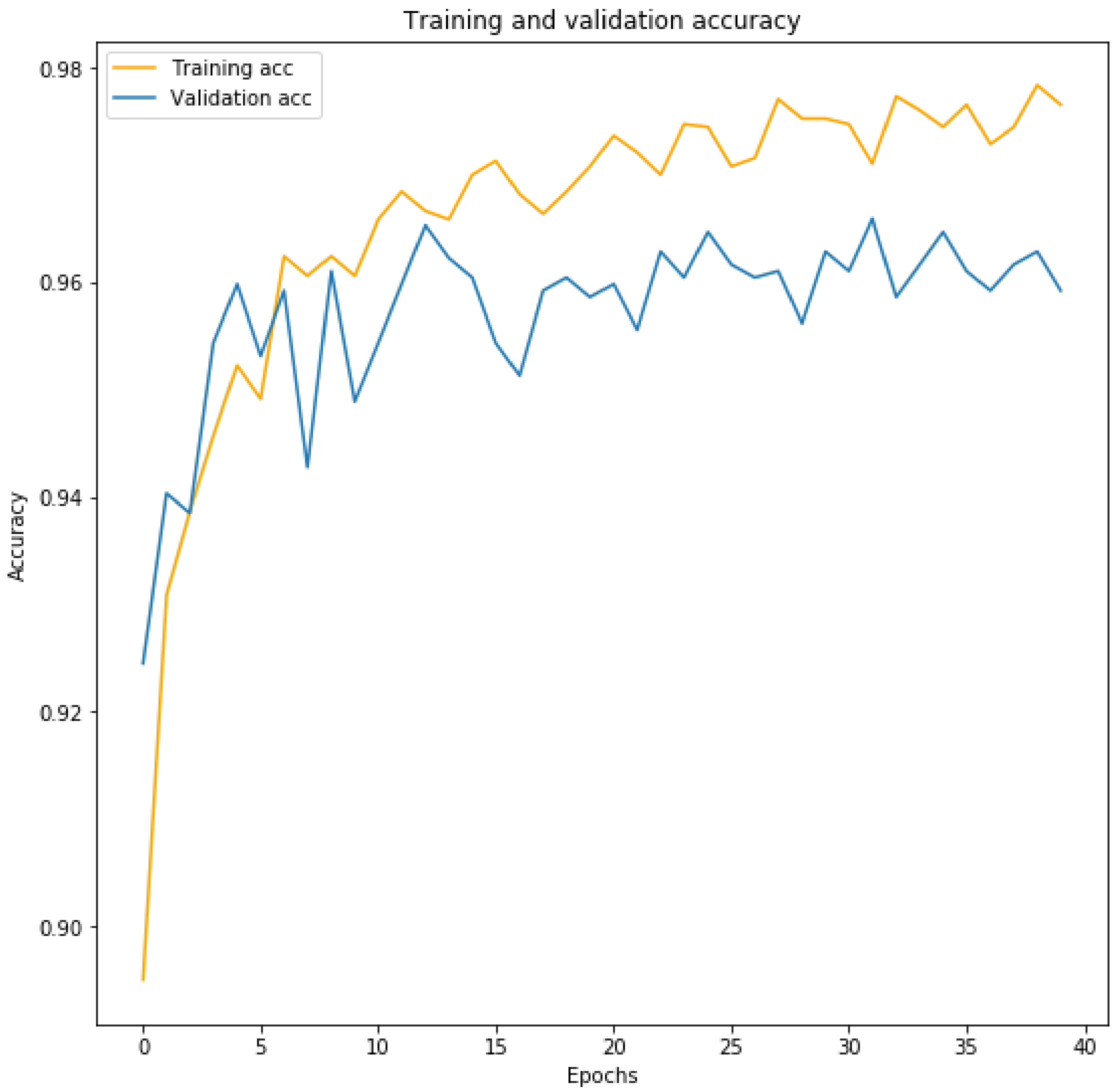
[66]:
```
model = models.Sequential()

model.add(layers.Conv1D(32, 3, activation='relu', input_shape=(10,1)))
model.add(layers.MaxPooling1D(2, padding="same"))
model.add(layers.Conv1D(64, 3, activation='relu', padding="same"))
model.add(layers.MaxPooling1D(2, padding="same"))
model.add(layers.Conv1D(128, 3, activation='relu', padding="same"))
model.add(layers.MaxPooling1D(2, padding="same"))
model.add(layers.Conv1D(128, 3, activation='relu', padding="same"))
model.add(layers.MaxPooling1D(2, padding="same"))
model.add(layers.Conv1D(128, 3, activation='relu', padding="same"))
model.add(layers.MaxPooling1D(2, padding="same"))
model.add(layers.Flatten())
model.add(layers.Dropout(0.5))
model.add(layers.Dense(300, activation="relu"))
model.add(layers.Dense(300, activation="relu"))
model.add(layers.Dense(6, activation="softmax"))
```

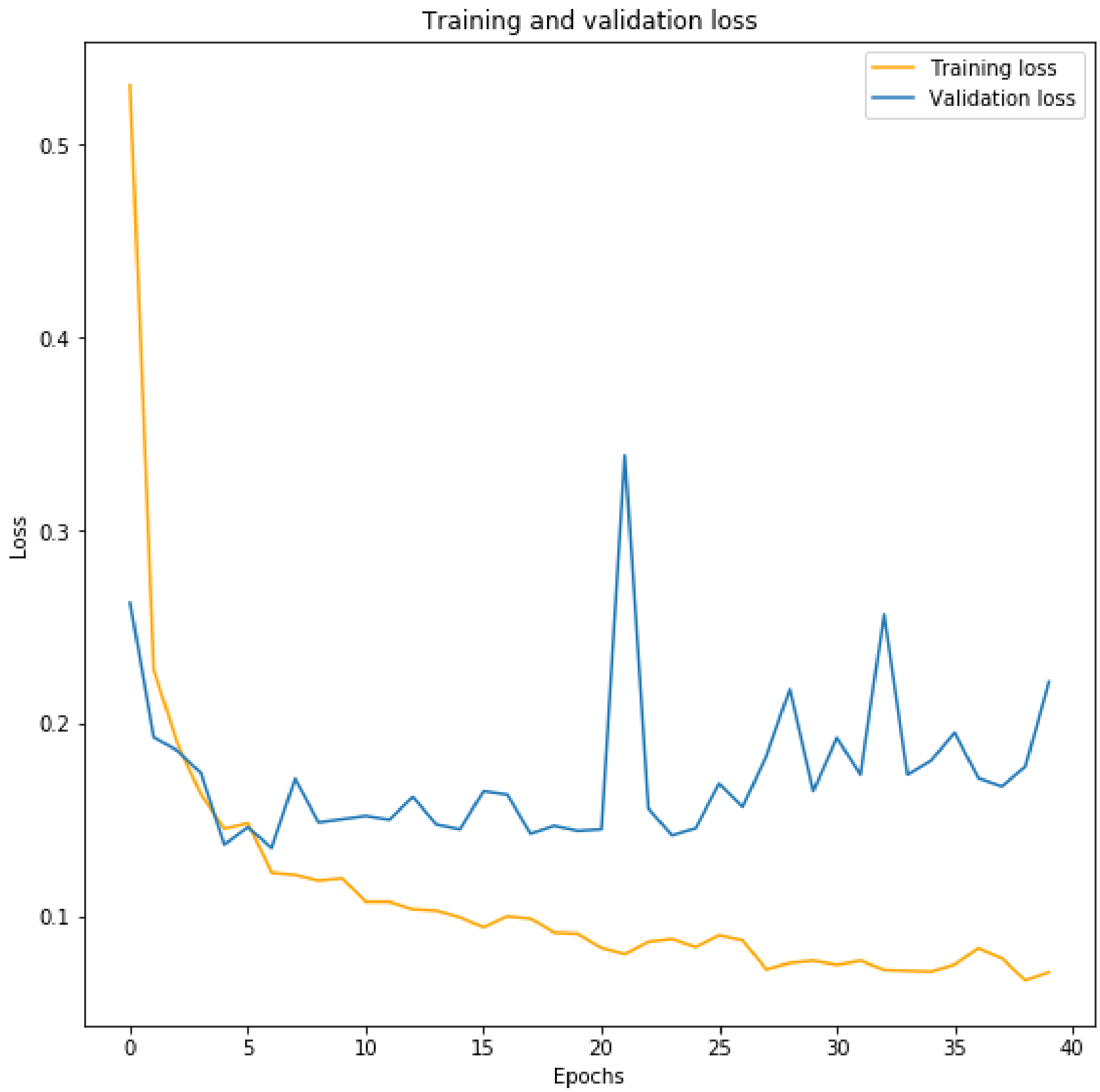
[67]:
```
model.compile(optimizer="adam",
              loss="categorical_crossentropy",
              metrics=["accuracy"])

model.summary()
```

```
Model: "sequential_2"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv1d_1 (Conv1D)            (None, 8, 32)             128
_________________________________________________________________
max_pooling1d_1 (MaxPooling1 (None, 4, 32)             0
_________________________________________________________________
conv1d_2 (Conv1D)            (None, 4, 64)             6208
_________________________________________________________________
max_pooling1d_2 (MaxPooling1 (None, 2, 64)             0
_________________________________________________________________
conv1d_3 (Conv1D)            (None, 2, 128)            24704
_________________________________________________________________
max_pooling1d_3 (MaxPooling1 (None, 1, 128)            0
_________________________________________________________________
conv1d_4 (Conv1D)            (None, 1, 128)            49280
_________________________________________________________________
max_pooling1d_4 (MaxPooling1 (None, 1, 128)            0
_________________________________________________________________
conv1d_5 (Conv1D)            (None, 1, 128)            49280
_________________________________________________________________
max_pooling1d_5 (MaxPooling1 (None, 1, 128)            0
_________________________________________________________________
flatten_1 (Flatten)          (None, 128)               0
_________________________________________________________________
dropout_4 (Dropout)          (None, 128)               0
_________________________________________________________________
dense_6 (Dense)              (None, 300)               38700
_________________________________________________________________
dense_7 (Dense)              (None, 300)               90300
_________________________________________________________________
dense_8 (Dense)              (None, 6)                 1806
=================================================================
Total params: 260,406
Trainable params: 260,406
Non-trainable params: 0
_________________________________________________________________
```

[68]:
```
hist = model.fit(X_train_tensor, y_train_ohe, epochs=40,␣
 ↪validation_data=(X_test_tensor, y_test_ohe), verbose=False)
```

[69]:
```
acc = hist.history['accuracy']
val_acc = hist.history['val_accuracy']
loss = hist.history['loss']
val_loss = hist.history['val_loss']

epochs = range(len(acc))

plt.figure(figsize=(9,9))
plt.plot(epochs, acc, color="orange", label='Training acc')
plt.plot(epochs, val_acc, label='Validation acc')
plt.ylabel("Accuracy")
plt.xlabel("Epochs")
plt.title('Training and validation accuracy')
plt.legend()

plt.figure(figsize=(9,9))
plt.plot(epochs, loss, color="orange", label='Training loss')
plt.plot(epochs, val_loss, label='Validation loss')
plt.ylabel("Loss")
plt.xlabel("Epochs")
plt.title('Training and validation loss')
plt.legend()

plt.show()
```


Training and validation accuracy
Training acc
Validation acc
Accuracy
Epochs
0.98
0.96
0.94
0.92
0.90
0
5
10
15
20
25
30
35
40



Looking at both curves we can see that the relatively complex model is overfitting.

[70]:
```
print(classification_report(model.predict_classes(X_test_tensor), y_test))
```

```
              precision    recall  f1-score   support

           1       0.99      0.97      0.98      1496
           2       0.80      0.94      0.87        90
           3       0.30      0.30      0.30        10
           4       0.68      0.78      0.72        27
           5       0.48      0.74      0.58        19

    accuracy                           0.96      1642
   macro avg       0.65      0.75      0.69      1642
```

```
weighted avg       0.96      0.96      0.96      1642
```

6 Conclusion

Though it took a lot longer to tune and train the MLPClassifier it definitly was worth it.

Compared to the Perceptron, RandomForst and XGBoost models it performs better in accuracy and F1 score.

By creating a neural network in Keras using Dense- and Dropout layers we could improve on the performance of the MLPClassifier and obtain a test accuracy of 96%. The F1-score also improved from 0.68 to 0.74. This results from a much better recall and only slightly worse precision of our custom Keras model.

By fitting a convolutional neural network we could even reach an accuracy score of 97%.