# Assignment2

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## 1 Assignment 2

1.0.1 Name: Yelisetty

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## 1.1 Importing Libraries

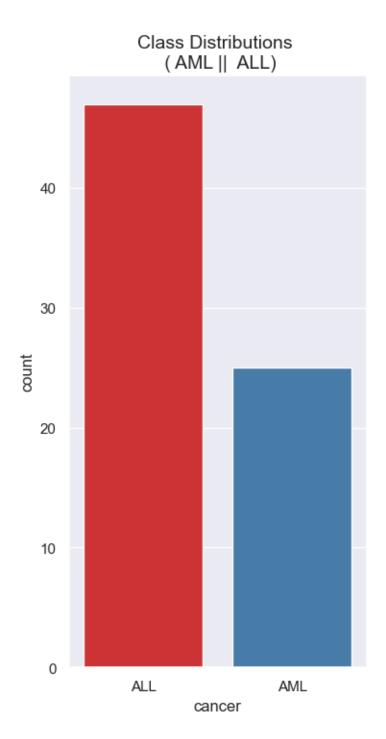
```
[2]: # Base libraries
     import pandas as pd
     import numpy as np
     from mpl toolkits.mplot3d import Axes3D
     import seaborn as sns; sns.set()
     import matplotlib.pyplot as plt
     %matplotlib inline
     # Preprocessing
     from sklearn.decomposition import PCA
     from sklearn.preprocessing import StandardScaler, scale
     # Models
     from sklearn.svm import SVC, LinearSVC
     from sklearn.ensemble import RandomForestClassifier
     from sklearn.neural_network import MLPClassifier
     from sklearn.feature_selection import SelectFromModel
     from sklearn.model_selection import GridSearchCV
     # Metrics
     from sklearn.metrics import confusion_matrix, accuracy_score, precision_score,
      ⇔recall_score, f1_score
```

## 1.2 Target Data

## 1.2.1 Loading dataset

```
[3]: cancer_targets = pd.read_csv("./data/Copy of actual.csv")
[4]: cancer_targets.head()
```

```
[4]:
       patient cancer
    0
              1
                   ALL
    1
              2
                   ALL
     2
              3
                   ALL
     3
              4
                   ALL
              5
     4
                   ALL
[5]: cancer_targets.dtypes
[5]: patient
                 int64
                object
    cancer
     dtype: object
    1.2.2 Class distribution
[6]: print(cancer_targets["cancer"].value_counts())
     print()
     print("Number of samples;", cancer_targets.shape)
    cancer
    ALL
           47
    AML
           25
    Name: count, dtype: int64
    Number of samples; (72, 2)
[7]: plt.figure(figsize=(4, 8))
     colors = ["AML", "ALL"]
     sns.countplot(data=cancer_targets, x='cancer', palette="Set1")
     plt.title('Class Distributions \n ( AML || ALL)', fontsize=14)
[7]: Text(0.5, 1.0, 'Class Distributions \n ( AML || ALL)')
```



#### 1.3 Train and test dataset

```
[8]: cancer_train = pd.read_csv("./data/data_train.csv")
     cancer_test = pd.read_csv("./data/data_test.csv")
     print("Train shape:", cancer_train.shape)
     print("Test shape:", cancer_test.shape)
     cancer_train.head(4)
    Train shape: (7129, 78)
    Test shape: (7129, 70)
[8]:
                           Gene Description Gene Accession Number
                                                                                2 \
                                                                      1 call
     O AFFX-BioB-5 at (endogenous control)
                                                   AFFX-BioB-5 at -214
                                                                           A -139
     1 AFFX-BioB-M_at (endogenous control)
                                                   AFFX-BioB-M_at -153
                                                                             -73
     2 AFFX-BioB-3_at (endogenous control)
                                                   AFFX-BioB-3 at -58
                                                                               -1
     3 AFFX-BioC-5_at (endogenous control)
                                                   AFFX-BioC-5_at
                                                                              283
                             4 call.3 ...
       call.1
                 3 call.2
                                           29 call.33
                                                        30 call.34
                                                                      31 call.35
     0
            A -76
                        A -135
                                    Α ...
                                           15
                                                    A -318
                                                                  A -32
                                                                               Α
                                                                  A -49
            A -49
                        A - 114
                                    A ... -114
                                                    A -192
     1
                                                                               Α
     2
                          265
                                                    A -95
                                                                    49
            A -307
                                            2
                                                                               Α
                                                                               Р
     3
             309
                            12
                                    A ... 193
                                                    A 312
                                                                  A 230
                      33 call.37
         32 call.36
     0 - 124
                  A -135
     1 -79
                  A -186
                               Α
     2 - 37
                  A -70
                               Α
     3 330
                  A 337
                               Α
```

[4 rows x 78 columns]

## 1.3.1 Preprocessing

We will be combining the train and test dataset for preprocessing and then we will split them again.

```
[9]: def rename_columns(df):
    for col in df.columns:
        if "call" in col:
            loc = df.columns.get_loc(col)
            patient = df.columns[loc-1]
            df.rename(columns={col: f'Call_{patient}'}, inplace=True)
```

```
[10]: rename_columns(df=cancer_train)
rename_columns(df=cancer_test)

cancer_train["Gene"] = cancer_train["Gene Description"] + \
```

## [10]: (144, 7130)

The columns labeled "Present," "Absent," and "Marginal" represent the detection calls made by the DNA Microarray manufacturer in the paper. These designations are based on comparing p-values of intensity calls to a predefined noise frequency cutoff. Consequently, it is advisable to remove rows where all values are designated as "Absent" (A) calls, as these are deemed unreliable.

Reference: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1409797/

## 1.3.2 Dropping the columns with all A in calls

```
[11]: call_rows = [row for row in df.index if "Call" in row]
  conditional = df.filter(call_rows, axis=0).apply(
        lambda x: x == 'A', axis=1).all()
  print(conditional.value_counts())
  df = df.loc[:, ~conditional]
```

False 5328
True 1802
Name: count, dtype: int64

## 1.3.3 Removing the call columns

```
[12]: df.drop(call_rows, axis=0, inplace=True)
    df['patient'] = df.index
    df['patient'] = df['patient'].astype('int')
    df.reset_index(drop=True)
```

```
[12]: Gene AFFX-BioC-5_at (endogenous control)_AFFX-BioC-5_at \
      1
                                                              283
      2
                                                              309
      3
                                                               12
      4
                                                              168
      67
                                                              141
      68
                                                               95
      69
                                                              146
      70
                                                              431
                                                                9
      71
      Gene hum_alu_at (miscellaneous control)_hum_alu_at
                                                      15091
      1
                                                      11038
      2
                                                      16692
      3
                                                      15763
      4
                                                      18128
      . .
                                                      22818
      67
      68
                                                      39323
      69
                                                      15689
      70
                                                      41570
      71
                                                      39538
      Gene AFFX-DapX-5_at (endogenous control)_AFFX-DapX-5_at
      0
      1
                                                               37
      2
                                                              183
      3
                                                               45
      4
                                                              -28
                                                                2
      67
      68
                                                              -26
      69
                                                                6
      70
                                                               94
      71
                                                             -104
      Gene AFFX-DapX-M_at (endogenous control)_AFFX-DapX-M_at
                                                              311
      1
                                                              134
      2
                                                              378
      3
                                                              268
      4
                                                              118
      67
                                                               46
```

```
68
                                                        73
69
                                                       302
70
                                                       235
71
                                                       101
Gene AFFX-LysX-5_at (endogenous control)_AFFX-LysX-5_at \
1
                                                       -21
2
                                                        67
3
                                                        43
4
                                                        -8
67
                                                        26
68
                                                        39
69
                                                        25
70
                                                        27
71
                                                       106
Gene AFFX-HUMISGF3A/M97935_MA_at (endogenous control)_AFFX-
HUMISGF3A/M97935_MA_at \
0
                                                       -13
1
                                                      -219
2
                                                       104
3
                                                      -148
                                                       -55
4
                                                       •••
67
                                                      -203
68
                                                       -60
69
                                                      -209
70
                                                      -626
71
                                                      -240
Gene AFFX-HUMISGF3A/M97935_MB_at (endogenous control)_AFFX-
HUMISGF3A/M97935_MB_at \
0
                                                       215
1
                                                       116
2
                                                       476
3
                                                       155
4
                                                       122
                                                       •••
67
                                                        25
68
                                                        60
69
                                                       183
70
                                                      -249
71
                                                       113
```

Gene AFFX-HUMISGF3A/M97935\_3\_at (endogenous control)\_AFFX-HUMISGF3A/M97935\_3\_at

```
\
                                                       797
0
                                                       433
1
2
                                                      1474
3
                                                       415
4
                                                       483
67
                                                       264
68
                                                       306
69
                                                       657
70
                                                       477
71
                                                      1313
Gene AFFX-HUMRGE/M10098_5_at (endogenous control)_AFFX-HUMRGE/M10098_5_at \
0
                                                     14538
1
                                                       615
2
                                                      5669
3
                                                      4850
4
                                                      1284
. .
67
                                                       104
68
                                                       569
69
                                                      3762
70
                                                      -159
71
                                                        34
Gene AFFX-HUMRGE/M10098_M_at (endogenous control)_AFFX-HUMRGE/M10098_M_at \
                                                      9738
1
                                                       115
2
                                                      3272
                                                      2293
3
4
                                                      2731
                                                       •••
67
                                                      -159
68
                                                       478
69
                                                      2164
70
                                                      -745
71
                                                       -62
Gene
     ... Transcription factor Stat5b (stat5b) mRNA_U48730_at \
1
                                                          169
2
                                                          315
3
                                                          240
4
                                                          156
. .
67
                                                           92
```

```
68
                                                           63
69
                                                          130
70
                                                           84
71
                                                           81
Gene Breast epithelial antigen BA46 mRNA_U58516_at \
                                                  511
1
                                                  837
2
                                                 1199
3
                                                  835
4
                                                  649
67
                                                  532
68
                                                  297
69
                                                  639
70
                                                 1141
71
                                                  574
Gene TUBULIN ALPHA-4 CHAIN_X06956_at \
                                   389
1
                                   442
2
                                   168
3
                                   174
4
                                   504
. .
67
                                   239
68
                                   358
69
                                   548
70
                                   197
71
                                   618
Gene PTGER3 Prostaglandin E receptor 3 (subtype EP3) {alternative
products}_X83863_at \
                                                       793
0
1
                                                       782
2
                                                      1138
3
                                                       627
4
                                                       250
. .
                                                       •••
67
                                                       707
68
                                                       423
69
                                                       809
70
                                                       466
71
                                                       551
Gene HMG2 High-mobility group (nonhistone chromosomal) protein 2_Z17240_at \
                                                       329
```

```
295
1
2
                                                        777
3
                                                        170
4
                                                        314
                                                        •••
                                                        354
67
68
                                                         41
69
                                                        445
70
                                                        349
71
                                                        194
Gene RB1 Retinoblastoma 1 (including osteosarcoma)_L49218_f_at \
1
                                                         11
2
                                                         41
3
                                                        -50
4
                                                         14
. .
                                                        -22
67
68
                                                          0
69
                                                         -2
70
                                                          0
71
                                                         20
Gene GB DEF = Glycophorin Sta (type A) exons 3 and 4; partial_M71243_f_at \
                                                        191
1
                                                         76
2
                                                        228
3
                                                        126
4
                                                         56
. .
67
                                                        260
68
                                                       1777
69
                                                        210
70
                                                        284
71
                                                        379
Gene GB DEF = mRNA (clone 1A7)_Z78285_f_at dataset patient
                                          -37
0
                                                train
                                                             1
1
                                          -14
                                                train
                                                             2
2
                                          -41
                                                train
                                                             3
                                          -91
3
                                                train
                                                             4
4
                                          -25
                                                train
                                                             5
                                            5
67
                                                            65
                                                 test
                                          -49
68
                                                            66
                                                  test
69
                                           16
                                                            63
                                                  test
```

```
1.3.4 Combining features and labels
[13]: df = pd.merge(left=df, right=cancer_targets,
                    left_on='patient', right_on='patient')
      print(df.shape)
      df.head(5)
     (72, 5330)
[13]:
        AFFX-BioC-5_at (endogenous control)_AFFX-BioC-5_at
                                                         283
      1
      2
                                                         309
      3
                                                          12
      4
                                                         168
        hum_alu_at (miscellaneous control)_hum_alu_at
      0
                                                  15091
                                                  11038
      1
      2
                                                  16692
      3
                                                  15763
                                                  18128
        AFFX-DapX-5_at (endogenous control)_AFFX-DapX-5_at
      0
      1
                                                          37
      2
                                                         183
      3
                                                          45
      4
                                                         -28
        AFFX-DapX-M_at (endogenous control)_AFFX-DapX-M_at
      0
                                                         311
                                                         134
      1
      2
                                                         378
      3
                                                         268
                                                         118
        AFFX-LysX-5_at (endogenous control)_AFFX-LysX-5_at
      1
                                                         -21
      2
                                                          67
      3
                                                          43
```

-73

-60

test

test

[72 rows x 5329 columns]

```
4
                                                    -8
 AFFX-HUMISGF3A/M97935_MA_at (endogenous control)_AFFX-HUMISGF3A/M97935_MA_at
\
0
                                                   -13
                                                  -219
1
2
                                                   104
3
                                                  -148
4
                                                   -55
 AFFX-HUMISGF3A/M97935_MB_at (endogenous control)_AFFX-HUMISGF3A/M97935_MB_at
/
0
                                                   215
1
                                                   116
2
                                                   476
3
                                                   155
4
                                                   122
 AFFX-HUMISGF3A/M97935_3_at (endogenous control)_AFFX-HUMISGF3A/M97935_3_at \
0
                                                   797
1
                                                   433
2
                                                  1474
3
                                                   415
4
                                                   483
 AFFX-HUMRGE/M10098_5_at (endogenous control)_AFFX-HUMRGE/M10098_5_at \
                                                 14538
1
                                                   615
2
                                                  5669
3
                                                  4850
4
                                                  1284
 AFFX-HUMRGE/M10098_M_at (endogenous control)_AFFX-HUMRGE/M10098_M_at ... \
0
                                                  9738
                                                   115
1
2
                                                  3272
                                                  2293
3
                                                  2731
 Breast epithelial antigen BA46 mRNA_U58516_at \
0
                                              837
1
2
                                             1199
3
                                              835
4
                                              649
```

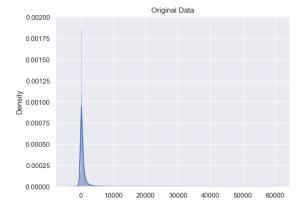
TUBULIN ALPHA-4 CHAIN\_X06956\_at \

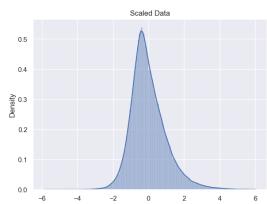
```
0
                               389
1
                               442
2
                               168
3
                               174
4
                               504
  PTGER3 Prostaglandin E receptor 3 (subtype EP3) {alternative
products}_X83863_at \
                                                   793
1
                                                   782
2
                                                  1138
3
                                                   627
                                                   250
  HMG2 High-mobility group (nonhistone chromosomal) protein 2_Z17240_at \
0
                                                   329
                                                   295
1
2
                                                   777
3
                                                   170
                                                   314
  RB1 Retinoblastoma 1 (including osteosarcoma)_L49218_f_at \
0
                                                    36
1
                                                    11
2
                                                    41
3
                                                   -50
                                                    14
  GB DEF = Glycophorin Sta (type A) exons 3 and 4; partial_M71243_f_at \
0
                                                   191
1
                                                    76
2
                                                   228
3
                                                   126
4
                                                    56
  GB DEF = mRNA (clone 1A7)_Z78285_f_at dataset patient cancer
0
                                      -37
                                            train
                                                        1
                                                              ALL
1
                                      -14
                                            train
                                                        2
                                                              ALL
2
                                      -41
                                            train
                                                         3
                                                              ALL
3
                                      -91
                                            train
                                                         4
                                                              ALL
                                      -25
                                                              ALL
                                            train
```

[5 rows x 5330 columns]

#### 1.3.5 Separate train and test data

```
[14]: train = df[df['dataset'] == 'train'].iloc[:, 0:-3]
      train_target = df[df['dataset'] == 'train'].iloc[:, -1]
      test = df[df['dataset'] == 'test'].iloc[:, 0:-3]
      test_target = df[df['dataset'] == 'test'].iloc[:, -1]
      print(train.shape, train_target.shape)
      print(test.shape, test_target.shape)
     (38, 5327) (38,)
     (34, 5327) (34,)
[15]: scaler = StandardScaler().fit(train)
      train_scaled = pd.DataFrame(scaler.transform(train), columns=train.columns)
      test_scaled = pd.DataFrame(scaler.transform(test), columns=test.columns)
      fig, ax = plt.subplots(ncols=2, figsize=(15, 5))
      sns.histplot(np.concatenate(train.values), ax=ax[0], kde=True, stat="density")
      sns.histplot(np.concatenate(train_scaled.values),
                   ax=ax[1], kde=True, stat="density")
      ax[0].set_title('Original Data')
      ax[1].set_title('Scaled Data')
      plt.tight_layout
      plt.show()
```





#### 1.3.6 Feature Selection

```
[16]: from sklearn.linear_model import LogisticRegression from sklearn.feature_selection import SelectFromModel print("Original Shape:", train_scaled.shape)
```

Original Shape: (38, 5327)

Features after selection using Logistic Regression: (38, 146)

/home/karthi/anaconda3/envs/ml/lib/python3.11/site-

packages/sklearn/linear\_model/\_sag.py:350: ConvergenceWarning: The max\_iter was reached which means the coef\_ did not converge

warnings.warn(

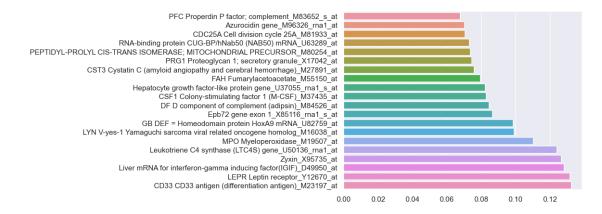
/home/karthi/anaconda3/envs/ml/lib/python3.11/site-packages/sklearn/base.py:457: UserWarning: X has feature names, but SelectFromModel was fitted without feature names

warnings.warn(

/home/karthi/anaconda3/envs/ml/lib/python3.11/site-packages/sklearn/base.py:457: UserWarning: X has feature names, but SelectFromModel was fitted without feature names

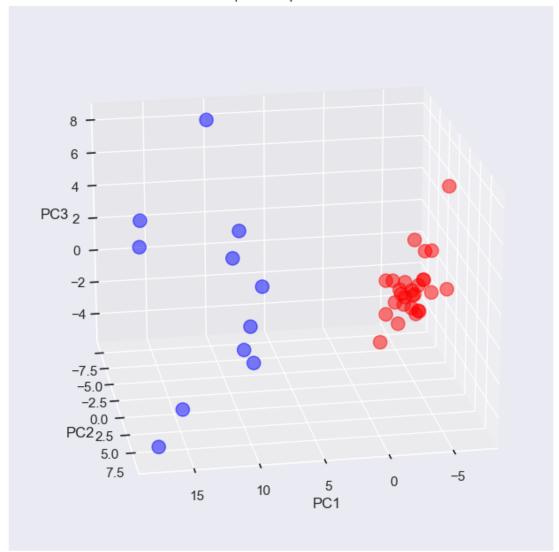
warnings.warn(

#### [16]: <Axes: >



## 1.3.7 Feature Scaling using PCA

[0.39758334 0.08187505 0.0603069 ]



First 3 Principal Components after PCA

# 2 Models being tested

- 1. C-Support Vector Classification (SVM)
- Using Grid search for tuning hyperparameters
- 2. Random forest Classifier
- Using Grid search for tuning hyperparameters
- 3. Neural Networks
- Using only Grid search

#### 2.1 SVM

## 2.1.1 Grid search for SVM

```
[19]: svc = SVC()
```

#### 2.1.2 Grid search parameters

## 2.1.3 Best parameters

```
[21]: grid.fit(train_scaled_logreg, train_target)
print(f"Best parameters for SVM are: {grid.best_params_}")
```

Best parameters for SVM are: {'C': 0.1, 'gamma': 1, 'kernel': 'linear'}

## 2.1.4 Selecting the best sym model

```
[22]: svc = grid.best_estimator_
```

#### 2.1.5 Fitting the model

```
[23]: svc.fit(train_scaled_logreg, train_target)
```

```
[23]: SVC(C=0.1, gamma=1, kernel='linear')
```

#### 2.1.6 Evaluation of the model

```
f"F1-score of the best SVM model is: {f1_score(test_target, test_pred, ⊔ →pos_label='AML')}")
```

```
TypeError
                                           Traceback (most recent call last)
/mnt/garuda/karthikeya/college/mlbio/Assignment2/Assignment2.ipynb Cell 46 line 1
      <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/</pre>
 Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=8'>9</a> print(
     <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/</pre>
 Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=9'>10</a>
                                                                       f"Recall c
 the best SVM model is: {recall_score(test_target, test_pred,__
 →pos_label='AML')}")
     <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/</pre>
 Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=10'>11</a> print(
     <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/</pre>
 -Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=11'>12</a>
                                                                        f"F1-scor
 of the best SVM model is: {f1_score(test_target, test_pred, pos_label='AML')}
     <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/</pre>
 Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=12'>13</a> print(
---> <a href='vscode-notebook-cell:/mnt/garuda/karthikeya/college/mlbio/
 →Assignment2/Assignment2.ipynb#Y600sZmlsZQ%3D%3D?line=13'>14</a>
                                                                        f"ROC-AUC
 score of the best SVM model is: {roc_auc_score(test_target, test_pred,__
 →pos label='AML')}")
File ~/anaconda3/envs/ml/lib/python3.11/site-packages/sklearn/utils/
 - param_validation.py:189, in validate_params.<locals>.decorator.<locals>.
 ⇔wrapper(*args, **kwargs)
    186 func sig = signature(func)
    188 # Map *args/**kwargs to the function signature
--> 189 params = func_sig.bind(*args, **kwargs)
    190 params.apply_defaults()
    192 # ignore self/cls and positional/keyword markers
File ~/anaconda3/envs/ml/lib/python3.11/inspect.py:3212, in Signature.bind(self
 →*args, **kwargs)
   3207 def bind(self, /, *args, **kwargs):
   3208
            """Get a BoundArguments object, that maps the passed `args`
   3209
            and `kwargs` to the function's signature. Raises `TypeError`
   3210
            if the passed arguments can not be bound.
            11 11 11
   3211
-> 3212
            return self._bind(args, kwargs)
File ~/anaconda3/envs/ml/lib/python3.11/inspect.py:3201, in Signature.
⇔ bind(self, args, kwargs, partial)
```

## 2.1.7 Plotting the confusion matrix

```
[]: # confusion matrix
cm = confusion_matrix(test_target, test_pred)

plt.figure(figsize=(5, 3))
sns.heatmap(cm, annot=True)
plt.xlabel('Predicted')
plt.ylabel('Truth')
plt.title('Confusion Matrix')
plt.show()
```

#### 2.2 Random Forest

## 2.2.1 Best parameters

```
[]: grid.fit(train_scaled_logreg, train_target)
print(f"Best parameters for Random Forest are: {grid.best_params_}")
```

## 2.2.2 Selecting the best random forest model

```
[]: rfc = grid.best_estimator_
```

## 2.2.3 Fitting the model

```
[]: rfc.fit(train_scaled_logreg, train_target)
```

## 2.2.4 Evaluation of the model

## 2.2.5 Plotting the confusion matrix

```
[]: # confusion matrix
cm = confusion_matrix(test_target, test_pred)

plt.figure(figsize=(5, 3))
sns.heatmap(cm, annot=True)
plt.xlabel('Predicted')
plt.ylabel('Truth')
plt.title('Confusion Matrix')
plt.show()
```

#### 2.3 Neural Network

#### 2.3.1 Grid search for MLP

```
[ ]: mlp = MLPClassifier(max_iter=1000)
```

## 2.3.2 Grid Parameters

```
'learning_rate': ['constant', 'adaptive']}
grid = GridSearchCV(mlp, param_grid, cv=3, scoring='accuracy')
```

## 2.3.3 Best parameters

```
[]: grid.fit(train_scaled_logreg, train_target)
print(f"Best parameters for Neural Network are: {grid.best_params_}")
```

## 2.3.4 Selecting the best neural network model

```
[]: mlp = grid.best_estimator_
```

## 2.3.5 Fitting the model

```
[]: mlp.fit(train_scaled_logreg, train_target)
```

## 2.3.6 Evaluating the model

#### 2.3.7 Plotting the confusion matrix

```
[]: # confusion matrix
cm = confusion_matrix(test_target, test_pred)

plt.figure(figsize=(5, 3))
sns.heatmap(cm, annot=True)
plt.xlabel('Predicted')
```

```
plt.ylabel('Truth')
plt.title('Confusion Matrix')
plt.show()
```