Task 2: Ensemble classifiers

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1 Introduction

For this assignment we be will employing predictive models based on decision trees to examine a dataset of cancer patients with the presence of 102 different peptides in the patients' organisms. The data is found in the files `cancerData.csv` and `cancerInfo.csv`.

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import sklearn
from sklearn.metrics import accuracy_score, zero_one_loss
from sklearn.metrics import confusion_matrix, classification_report,␣
 ↪ConfusionMatrixDisplay
from sklearn.model_selection import GridSearchCV
```

2 Exploratory Data Analysis

We first import the data and analyse its structure. We can immediately see that the data ingestion pipeline will require some work.

[2]:
```
df1 = pd.read_csv("cancerDat.csv", sep = ";", decimal = ",")
df1 = df1.T
df1 = df1.drop('Unnamed: 0', axis=0)
```

```
display(df1.head())
print(df1.shape)
```

```
                 0          1          2          3          4          5    \
NO.REC_1  21.923472  24.442617  19.050562  18.482667  24.086793   20.32946
NO.REC_2  21.020165  23.649841  18.402413  19.088996  24.710323  21.495392
NO.REC_3  19.585788  23.736128  18.191527   16.33124  21.917326  20.284533
NO.REC_4  19.061767  23.374865  17.692775   15.36272  21.484924  18.379603
NO.REC_5  18.547029  23.039588  19.066973  15.835721  21.339587  19.550809

                 6          7          8          9    ...        92   \
NO.REC_1  19.304363  24.270429  18.878984  18.752264  ...  19.439382
NO.REC_2  19.454826  25.807051  19.091796  19.213397  ...  20.631064
NO.REC_3  16.853825  22.661125  18.215654  20.821777  ...  19.123832
NO.REC_4  16.513507  21.401436   18.38696  19.847221  ...  17.958307
NO.REC_5  16.831653  21.776832   17.85408  20.368534  ...  18.212854

                 93         94         95         96         97         98   \
NO.REC_1  16.142102  22.858297  22.262118  18.079186  17.151515  20.912124
NO.REC_2        NaN  22.028998  22.031468  17.101384  18.315637  21.512601
NO.REC_3  16.171227  23.143305  22.334392  17.159968  16.859732  19.076147
NO.REC_4        NaN  19.183961  17.851328  16.564709  15.161135  18.190653
NO.REC_5        NaN  22.228449  21.385404  17.072001  15.071656  18.896095

                 99         100        101
NO.REC_1  17.298159  19.097263   21.21211
NO.REC_2  17.100711  18.875548  23.980238
NO.REC_3  15.417028  16.340283  19.810886
NO.REC_4  15.269443  15.411408  18.351433
NO.REC_5  15.147357        NaN   20.28779

[5 rows x 102 columns]

(129, 102)
```

```
[3]: df2 = pd.read_csv("cancerInfo.csv", sep = ";")
     df2 = df2.drop(['Unnamed: 0', 'Group'], axis = 1)
     df2.index = df2.iloc[:,0]
     df2 = df2.drop(['sampleNames'], axis = 1)
     display(df2.head())
```

```
            sites
sampleNames
NO.REC_1        A
NO.REC_2        B
NO.REC_3        C
NO.REC_4        C
NO.REC_5        C
```

We want to define a single response variable according to whether the cancer sees a recurrence or not. This is currently coded into the key of the patient, so we will create a separate binary vector to encode this response, where `0` will denote non-recurrence and `1` will denote recurrence.

[4]:
```
indices1 = np.array(df1.index).astype(str)
index_array1 = np.zeros(len(indices1))
labels_1 = np.where(np.char.startswith(indices1, 'NO.REC_'), 0, np.where(np.char.
 ↪startswith(indices1, 'REC_'), 1, index_array1))

indices2 = np.array(df2.index).astype(str)
index_array2 = np.zeros(len(indices2))
labels_2 = np.where(np.char.startswith(indices2, 'NO.REC_'), 0, np.where(np.char.
 ↪startswith(indices2, 'REC_'), 1, index_array2))

print("Labels are equal: " + str(np.array_equal(labels_1, labels_2))) # That is␣
 ↪we can define a single response variable y for the two files
y = labels_1
```

```
Labels are equal: True
```

[5]:
```
y = pd.Series(y)
display(y)
```

```
0      0.0
1      0.0
2      0.0
3      0.0
4      0.0
      ...
124    1.0
125    1.0
126    1.0
127    1.0
128    1.0
Length: 129, dtype: float64
```

Now we will check for missing values and some descriptive statistics of the data. There is a substantial amount of missing values in the dataset, so in order to avoid discarding such a large amount of information, we resort to imputing the linear interpolation of the missing entries. This increases the amount of information that we work with, but we claim that for the final results this is preferable to eliminating the entire rows and rendering our dataset almost empty.

[6]:
```
for col in df1:
    df1[col] = pd.to_numeric(df1[col], errors='coerce')
df1.dtypes
```

[6]:
```
0      float64
1      float64
```

```
2      float64
3      float64
4      float64
        ...
97     float64
98     float64
99     float64
100    float64
101    float64
Length: 102, dtype: object
```

[7]:
```
print(df1.isnull().values.any())
print(sum(df1.isnull()))
df1 = df1.interpolate(method ='linear', limit_direction ='forward')
print(df1.isnull().values.any())
```

```
True
5151
False
```

[8]:
```
print(df2.isnull().values.any()) # False -> No nulls
```

```
False
```

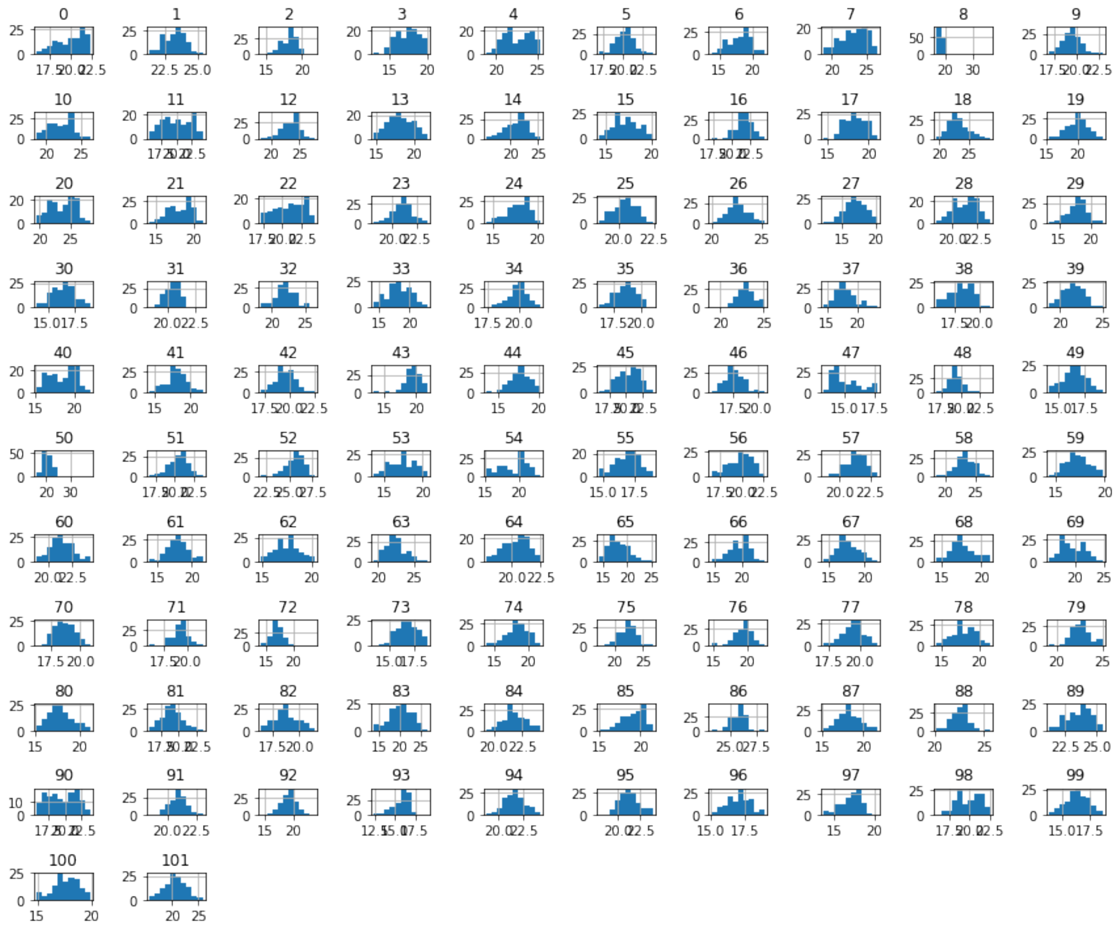
Now that we have handled the missing values, we can go ahead and perform some more sophisticated exploration techniques.

[9]:
```
df1.describe()
```

[9]:
```
                0           1           2           3           4           5    \
count  129.000000  129.000000  129.000000  129.000000  129.000000  129.000000
mean    19.930039   23.286214   18.226328   17.331228   22.591467   20.193446
std      1.646143    0.784218    1.126192    1.477403    1.562914    1.185180
min     15.836862   21.313713   14.401524   12.976690   18.807566   16.963778
25%     18.547029   22.755110   17.440432   16.166380   21.321595   19.397560
50%     20.341514   23.374865   18.349787   17.373647   22.461809   20.264099
75%     21.362745   23.793517   18.968572   18.501081   23.992847   20.961033
max     22.315946   25.387870   21.837865   19.994349   25.306821   23.671558

                6           7           8           9    ...          92   \
count  129.000000  129.000000  129.000000  129.000000  ...  129.000000
mean    18.133973   23.193300   18.687522   19.516615  ...   19.126770
std      1.751196    1.860021    1.744740    1.068425  ...    1.399915
min     13.770822   18.824646   16.818849   16.952402  ...   14.488970
25%     17.001766   22.036426   18.109188   18.830477  ...   18.323381
50%     18.421874   23.469361   18.548956   19.546749  ...   19.240883
75%     19.426085   24.633681   18.967436   20.108405  ...   19.956155
max     21.934433   26.596796   36.306672   22.920624  ...   23.668357
```

```
              93          94          95          96          97          98  \
count  129.000000  129.000000  129.000000  129.000000  129.000000  129.000000
mean    15.832452   21.643638   21.312564   17.060424   17.096818   19.891371
std      1.005218    1.009982    1.126496    0.881310    1.241427    1.487108
min     12.398937   18.802740   17.851328   15.050081   13.746502   15.860695
25%     15.358616   20.940953   20.538005   16.466670   16.297205   18.855134
50%     16.099669   21.663512   21.281094   17.156167   17.270199   19.892329
75%     16.514396   22.295952   22.004275   17.734682   18.003294   21.065003
max     19.057885   24.195671   23.932574   19.008904   20.339064   22.552429

              99         100         101
count  129.000000  129.000000  129.000000
mean    16.372295   17.653626   20.692479
std      1.011885    1.123423    2.025807
min     13.846473   14.930870   15.644922
25%     15.707511   17.008565   19.477624
50%     16.416639   17.691291   20.655011
75%     17.101205   18.540819   22.009082
max     18.586913   19.888654   25.794838

[8 rows x 102 columns]
```

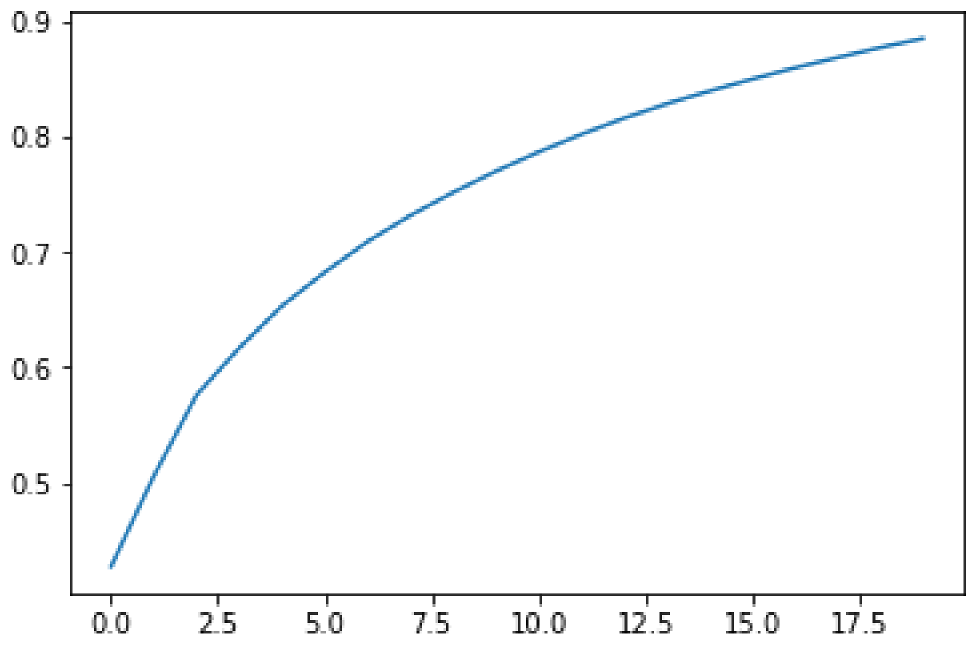
[10]:
```
df1.hist(figsize=(12,10))
plt.tight_layout()
plt.show()
```



In the previous cells, we can observe some erratic distributions for some of the covariates, where they do not seem to fit very well with the statement of the law of large numbers. Specifically, as an example, the covariates indexed in positions `15`, `54` or `78` have some interesting shapes.

[11]:
```python
from sklearn.decomposition import PCA
import itertools
pca = PCA(n_components=20)
pca.fit_transform(df1)
#print(pca.explained_variance_ratio_)
#print(list(itertools.accumulate(pca.explained_variance_ratio_)))
plt.plot(list(itertools.accumulate(pca.explained_variance_ratio_)))
```

[11]:
```
[<matplotlib.lines.Line2D at 0x779719e76560>]
```



We can see from the PCA that the amount of variance accumulated by the twenty first principal components amounts to almost 90%. Our final classifiers will only include ten peptides as features to train on.

3 Train-Test Split

[12]:
```python
from sklearn.model_selection import train_test_split
np.random.seed(1234)
```

We separate the data into two sets: the training set and the test set.

[13]:
```python
X_train, X_test, y_train, y_test = train_test_split(
                                        df1,
                                        y,
                                        test_size = 1/3,
                                        random_state = 1234)
```

[14]:
```python
print(X_train.shape, X_test.shape, y_train.shape, y_test.shape)
```

```
(86, 102) (43, 102) (86,) (43,)
```

4 Model fitting

We'll fit the following models: a Random Forest Classifier and two Boosting Classifiers.

4.1 Random Forest Classifier

```
[15]: from sklearn.ensemble import RandomForestClassifier
      rf = RandomForestClassifier(random_state = 1234)
      parameters = {'n_estimators' : range(10,130,20),
                    'max_features' : (1,2,3,4,5,6,7,8,9,10)
                   }
```

We implement a grid search procedure.

```
[16]: grid_rf = GridSearchCV(rf, parameters)
      grid_rf.fit(X_train, y_train)
```

```
[16]: GridSearchCV(estimator=RandomForestClassifier(random_state=1234),
                   param_grid={'max_features': (1, 2, 3, 4, 5, 6, 7, 8, 9, 10),
                               'n_estimators': range(10, 130, 20)})
```

```
[17]: rf_results = pd.DataFrame(grid_rf.cv_results_)
      rf_results.filter(regex = '(param.*|mean_t|std_t)') \
          .drop(columns = 'params') \
          .sort_values('mean_test_score', ascending = False) \
          .head(4)
```

```
[17]:    param_max_features param_n_estimators  mean_test_score  std_test_score
      36                  7                 10         0.594118        0.118234
      55                 10                 30         0.582353        0.079792
      48                  9                 10         0.572549        0.142693
      1                   1                 30         0.569935        0.044213
```

```
[18]: best_params = grid_rf.best_params_
      print("Best Parameters:", best_params)
      best_rf = RandomForestClassifier(**best_params, random_state=1234)
      best_rf.fit(X_train, y_train)
```

```
Best Parameters: {'max_features': 7, 'n_estimators': 10}
```

```
[18]: RandomForestClassifier(max_features=7, n_estimators=10, random_state=1234)
```

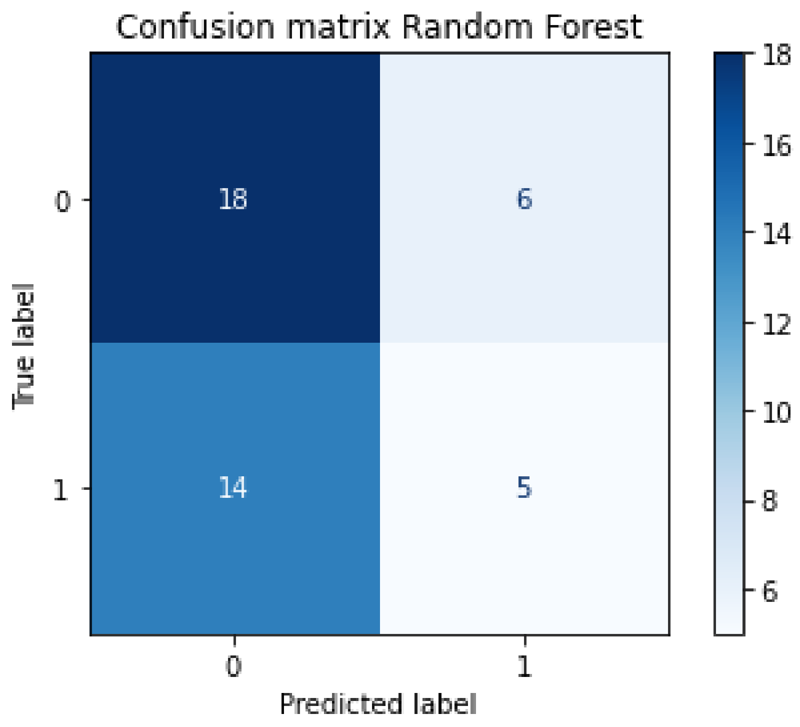
The accuracy and performance of RF is as follows.

```
[19]: y_pred = best_rf.predict(X_test)
      accuracy_score(y_pred, y_test)
```

```
[19]: 0.5348837209302325
```

```
[20]: confusion_mtx = confusion_matrix(y_test, y_pred)
      disp = ConfusionMatrixDisplay(confusion_matrix= confusion_mtx, display_labels=␣
       ↪None)
```

```
disp.plot(cmap= plt.cm.Blues)
plt.title("Confusion matrix Random Forest")
plt.show()
```



Finally, the most relevant variables in the prediction are given by the following code:

```
[21]: feature_importances = best_rf.feature_importances_
importance_df = pd.DataFrame({'Feature' : X_train.columns, 'Importance' :␣
 ↪feature_importances})
print(importance_df.sort_values(by=['Importance'], ascending=False).head(10))
```

```
    Feature  Importance
51       51    0.057151
11       11    0.043937
25       25    0.032852
96       96    0.030232
78       78    0.029687
76       76    0.028671
5         5    0.027653
34       34    0.026475
12       12    0.026456
62       62    0.024448
```

4.2 Gradient Boosting

Using stumps as classification trees for the response variable, we compute the misclassification rates of both the learning set and the test set across 2,000 iterations.

```
[22]: from sklearn.ensemble import GradientBoostingClassifier
      gb = GradientBoostingClassifier(n_estimators=2000, random_state=1234)
      parameters = {'max_depth' : (1,4,8,16)}
```

```
[23]: grid_gb = GridSearchCV(gb, parameters)
      grid_gb.fit(X_train, y_train)
```

```
[23]: GridSearchCV(estimator=GradientBoostingClassifier(n_estimators=2000,
                                                        random_state=1234),
                   param_grid={'max_depth': (1, 4, 8, 16)})
```

The results of comparing the test-set misclassification rates attained by different ensemble classifiers based on trees with varying maximum depth is shown in the following table.

```
[24]: gb_results = pd.DataFrame(grid_gb.cv_results_)
      gb_results.filter(regex = '(param.*|mean_t|std_t)') \
          .drop(columns = 'params') \
          .sort_values('mean_test_score', ascending = False) \
          .head(4)
```

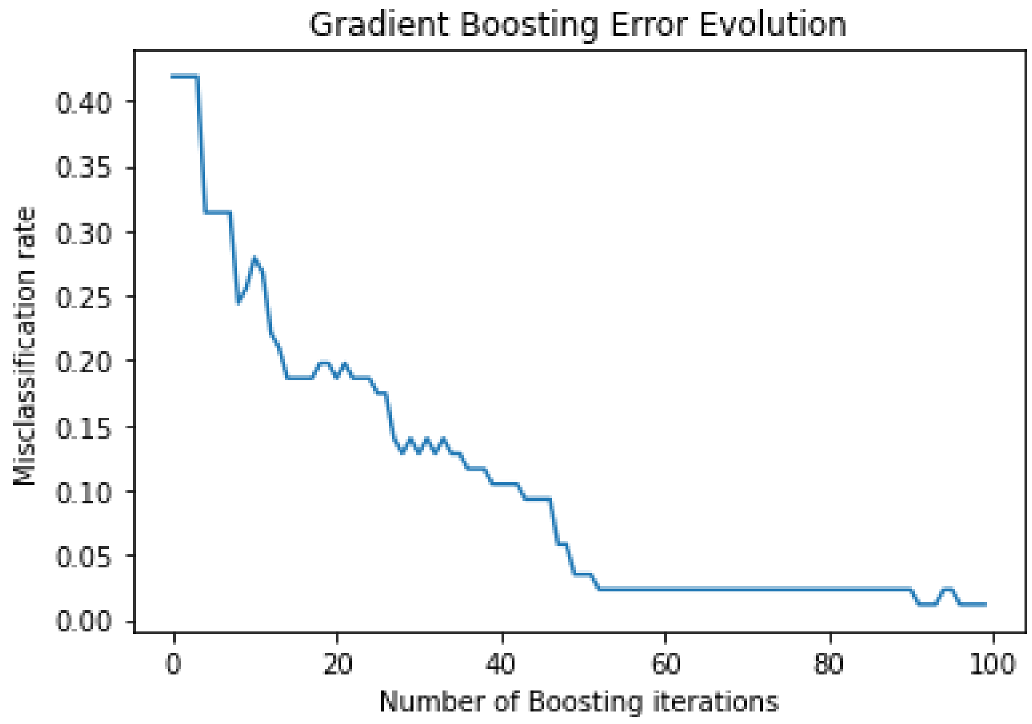
```
[24]:   param_max_depth  mean_test_score  std_test_score
      0               1         0.524183        0.069834
      2               8         0.454248        0.103714
      3              16         0.454248        0.103714
      1               4         0.442484        0.090319
```

The following plot represents graphically the error as a function of the number of boosting iterations.

```
[25]: best_params = grid_gb.best_params_
      print("Best Parameters:", best_params)

      train_errors = []
      best_gb = GradientBoostingClassifier(**best_params, random_state=1234)
      best_gb.fit(X_train, y_train)

      for i, y_pred_train in enumerate(best_gb.staged_predict(X_train)):
          train_errors.append(zero_one_loss(y_train, y_pred_train))

      plt.plot(np.arange(0,100), train_errors)
      plt.xlabel('Number of Boosting iterations')
      plt.ylabel('Misclassification rate')
      plt.title('Gradient Boosting Error Evolution')
```

```
Best Parameters: {'max_depth': 1}
```

[25]:
```
Text(0.5, 1.0, 'Gradient Boosting Error Evolution')
```

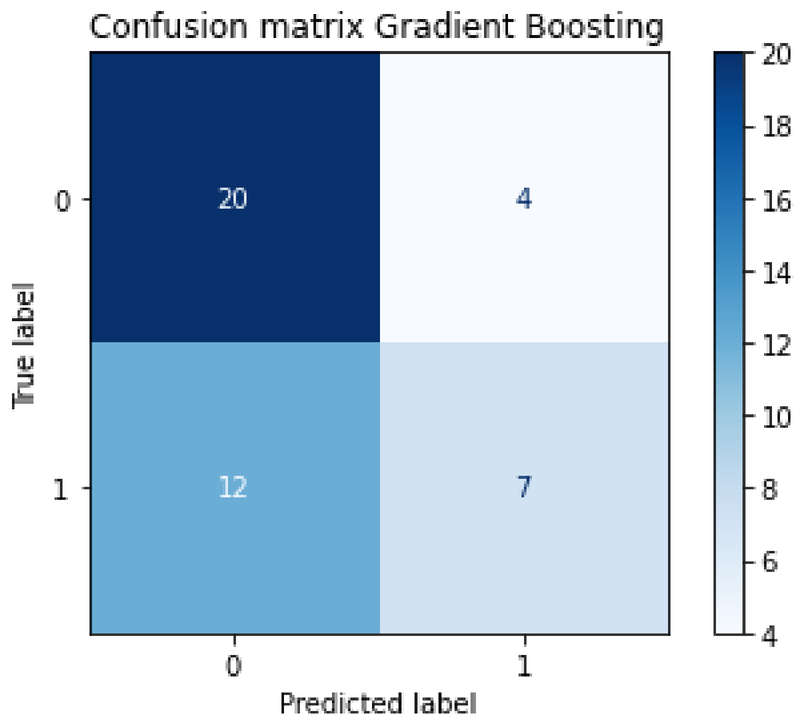


The accuracy and performance of Gradient Boosting is as follows.

[34]:
```
y_pred = best_gb.predict(X_test)
accuracy_score(y_pred, y_test)
```

[34]:
```
0.627906976744186
```

[35]:
```
confusion_mtx = confusion_matrix(y_test, y_pred)
disp = ConfusionMatrixDisplay(confusion_matrix= confusion_mtx, display_labels=␣
 ↪None)
disp.plot(cmap= plt.cm.Blues)
plt.title("Confusion matrix Gradient Boosting")
plt.show()
```



4.3 XGBoost

To conclude, we introduce another boosting flavour and analyse its performance.

[36]:
```
import xgboost
xgb = xgboost.XGBClassifier(n_estimators=2000, random_state=1234)
parameters = {'max_depth' : (1,4,8,16),
              'learning_rate' : [0,2]
              }
```

[37]:
```
grid_xgb = GridSearchCV(xgb, parameters)
grid_xgb.fit(X_train, y_train)
```

[37]:
```
GridSearchCV(estimator=XGBClassifier(base_score=None, booster=None,
                                     callbacks=None, colsample_bylevel=None,
                                     colsample_bynode=None,
                                     colsample_bytree=None, device=None,
                                     early_stopping_rounds=None,
                                     enable_categorical=False, eval_metric=None,
                                     feature_types=None, gamma=None,
                                     grow_policy=None, importance_type=None,
                                     interaction_constraints=None,
                                     learning_rate=None, max_bin=None,
                                     max_cat_threshold=None,
                                    max_cat_to_onehot=None,
                                    max_delta_step=None, max_depth=None,
                                    max_leaves=None, min_child_weight=None,
                                    missing=nan, monotone_constraints=None,
                                    multi_strategy=None, n_estimators=2000,
                                    n_jobs=None, num_parallel_tree=None,
                                    random_state=1234, ...),
             param_grid={'learning_rate': [0, 2], 'max_depth': (1, 4, 8, 16)})
```

[38]:
```python
xgb_results = pd.DataFrame(grid_xgb.cv_results_)
xgb_results.filter(regex = '(param.*|mean_t|std_t)') \
    .drop(columns = 'params') \
    .sort_values('mean_test_score', ascending = False) \
    .head(4)
```

[38]:
```
  param_learning_rate param_max_depth  mean_test_score  std_test_score
0                   0               1         0.581699        0.013072
1                   0               4         0.581699        0.013072
2                   0               8         0.581699        0.013072
3                   0              16         0.581699        0.013072
```

[39]:
```python
best_params = grid_xgb.best_params_
print("Best Parameters:", best_params)

best_xgb = xgboost.XGBClassifier(**best_params, random_state=1234)
best_xgb.fit(X_train, y_train)
```

```
Best Parameters: {'learning_rate': 0, 'max_depth': 1}
```

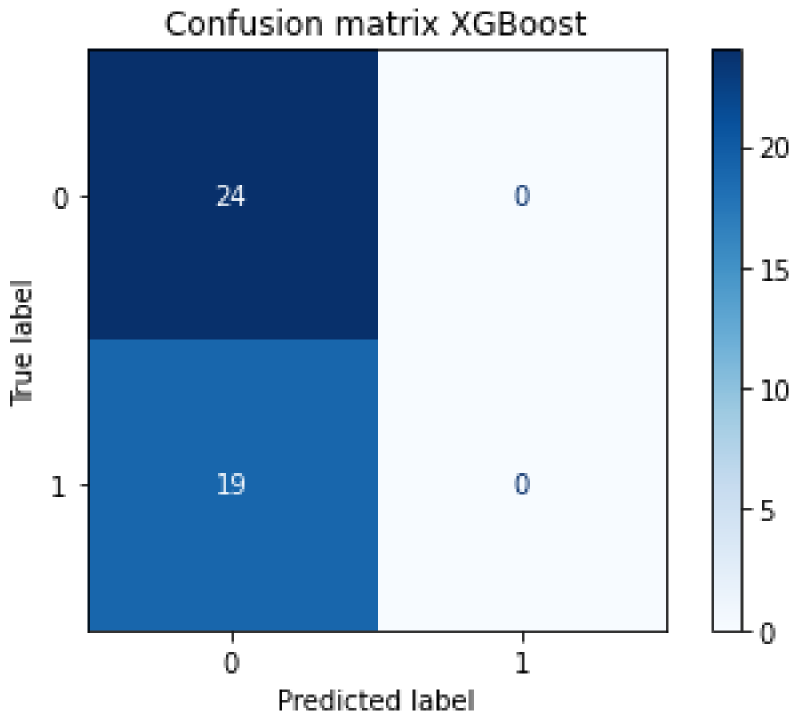
[39]:
```
XGBClassifier(base_score=None, booster=None, callbacks=None,
              colsample_bylevel=None, colsample_bynode=None,
              colsample_bytree=None, device=None, early_stopping_rounds=None,
              enable_categorical=False, eval_metric=None, feature_types=None,
              gamma=None, grow_policy=None, importance_type=None,
              interaction_constraints=None, learning_rate=0, max_bin=None,
              max_cat_threshold=None, max_cat_to_onehot=None,
              max_delta_step=None, max_depth=1, max_leaves=None,
              min_child_weight=None, missing=nan, monotone_constraints=None,
              multi_strategy=None, n_estimators=None, n_jobs=None,
              num_parallel_tree=None, random_state=1234, ...)
```

The accuracy and performance of XGBoost is as follows.

[40]:
```python
y_pred = best_xgb.predict(X_test)
accuracy_score(y_pred, y_test)
```

[40]:
```
0.5581395348837209
```

[41]:
```
confusion_mtx = confusion_matrix(y_test, y_pred)
disp = ConfusionMatrixDisplay(confusion_matrix= confusion_mtx, display_labels=␣
 ↪None)
disp.plot(cmap= plt.cm.Blues)
plt.title("Confusion matrix XGBoost")
plt.show()
```



We can see how the gradient boosting always predicts the most common class, and so has a large amount of Type 1 errors.

5 Predictor comparison

The accuracies of the three proposed models are the following:

[45]:
```
print("Accuracy of RF:", accuracy_score(best_rf.predict(X_test), y_test))
print("Accuracy of GB:", accuracy_score(best_gb.predict(X_test), y_test))
print("Accuracy of XGB:", accuracy_score(best_xgb.predict(X_test), y_test))
```

```
Accuracy of RF: 0.5348837209302325
Accuracy of GB: 0.627906976744186
Accuracy of XGB: 0.5581395348837209
```

We can see that, in general, they're not very high. This can be due to the number of NaNs in the data used. However, the Gradient Boosting method obtains a result considerably better than the other two methods, followed by the XGB and then the RF, which obtain similar results. For this reason, the classifier we would choose would be Gradient Boosting.

Using Gradient Boosting, the ten most relevant recurrence biomarkers are the following peptides:

```
[46]: feature_importances = best_gb.feature_importances_
      importance_gb = pd.DataFrame({'Feature' : X_train.columns, 'Importance' :␣
       ↪feature_importances})
      print(importance_gb.sort_values(by=['Importance'], ascending=False).head(10))
```

```
    Feature  Importance
51       51    0.123774
11       11    0.112551
65       65    0.089577
60       60    0.067424
38       38    0.067323
70       70    0.067106
76       76    0.058383
19       19    0.048530
75       75    0.036543
67       67    0.032089
```