Wine type prediction project prepared by: Ahmed Ayari & Amira Dridi

Our project steps:

1) *Data understanding and visualization*
2) *Data preprocessing*
3) *Train and test data preparation*
4) *Implementation and evaluation of machine learning models (Xgboost and random forest)*
5) *Implementation of the neural network model*
6) *Training and evaluating the model*
7) *Conclusion*

1) Data understanding

```
red_wine_data.head()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	5
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.8	5
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.8	5
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.8	6
4	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4	5

```
[69] red_wine_data.shape
```

```
(1599, 12)
```

```
[ ] white_wine_data.head()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	6
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	6
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	6
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6

```
white_wine_data.shape
```

```
(4898, 12)
```

```
[53] # Concat datasets with the right wine_type
     white_wine_data['wine_type'] = 1
     red_wine_data['wine_type'] = 0
     datasets = [red_wine_data,white_wine_data]
     wine_data = pd.concat(datasets,ignore_index=True)
```

```
[55] wine_data.shape
```

```
(6497, 13)
```

```
wine_data.describe()
```

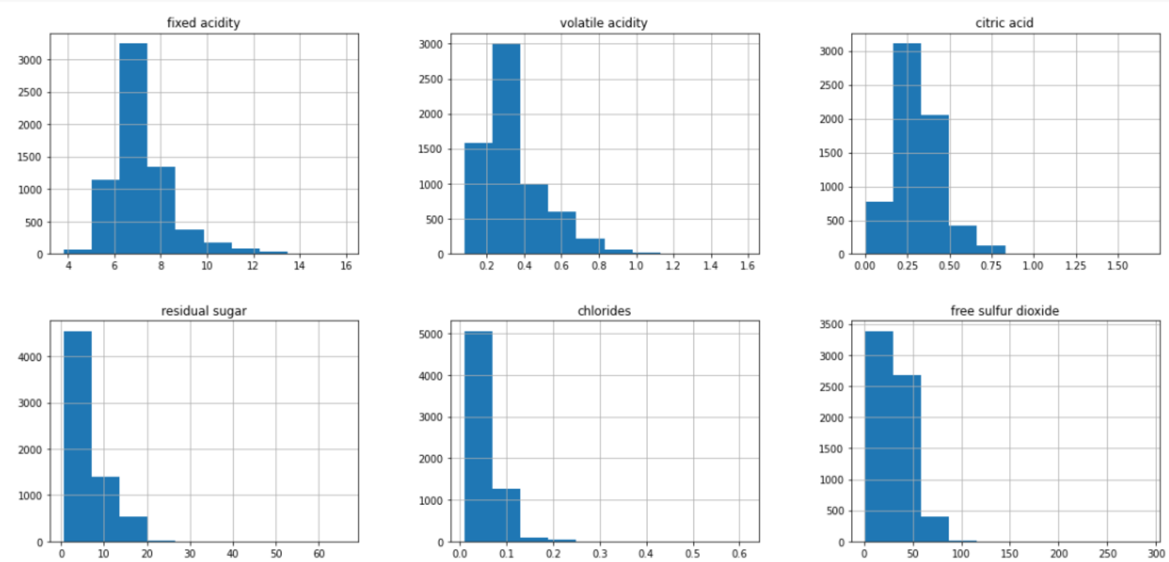
	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
count	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000	6497.000000
mean	7.215307	0.339666	0.318633	5.443235	0.056034	30.525319	115.744574	0.994697	3.218501	0.531268	10.491801	5.818378
std	1.296434	0.164636	0.145318	4.757804	0.035034	17.749400	56.521855	0.002999	0.160787	0.148806	1.192712	0.873255
min	3.800000	0.080000	0.000000	0.600000	0.009000	1.000000	6.000000	0.987110	2.720000	0.220000	8.000000	3.000000
25%	6.400000	0.230000	0.250000	1.800000	0.038000	17.000000	77.000000	0.992340	3.110000	0.430000	9.500000	5.000000
50%	7.000000	0.290000	0.310000	3.000000	0.047000	29.000000	118.000000	0.994890	3.210000	0.510000	10.300000	6.000000
75%	7.700000	0.400000	0.390000	8.100000	0.065000	41.000000	156.000000	0.996990	3.320000	0.600000	11.300000	6.000000
max	15.900000	1.580000	1.660000	65.800000	0.611000	289.000000	440.000000	1.038980	4.010000	2.000000	14.900000	9.000000

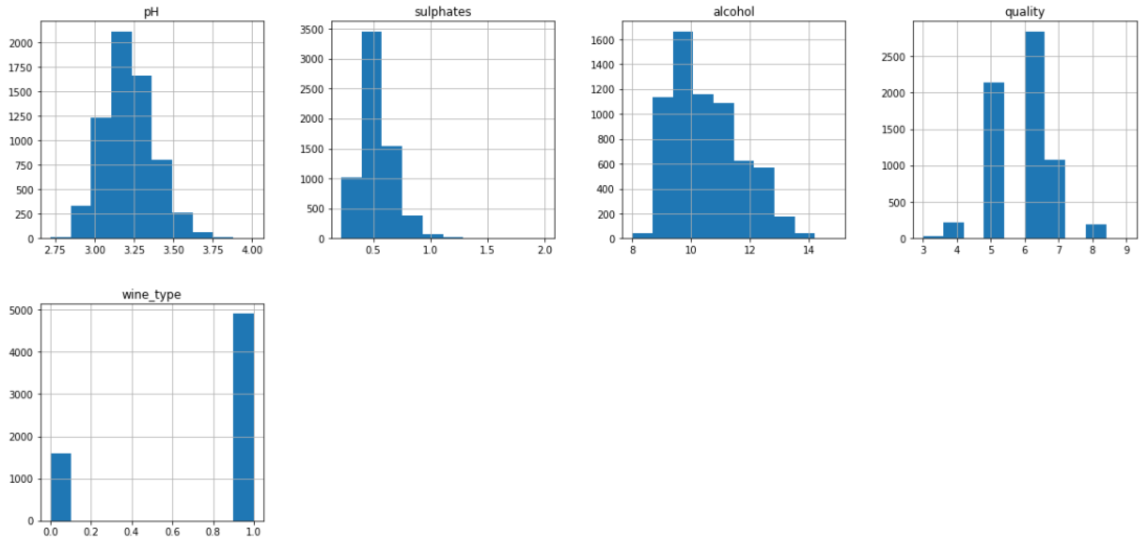
```
wine_data.isnull().sum()
```

```
fixed acidity           0
volatile acidity        0
citric acid             0
residual sugar          0
chlorides               0
free sulfur dioxide     0
density                 0
pH                      0
sulphates               0
alcohol                 0
quality                 0
wine type               0
dtype: int64
```

- *Data visualization:*

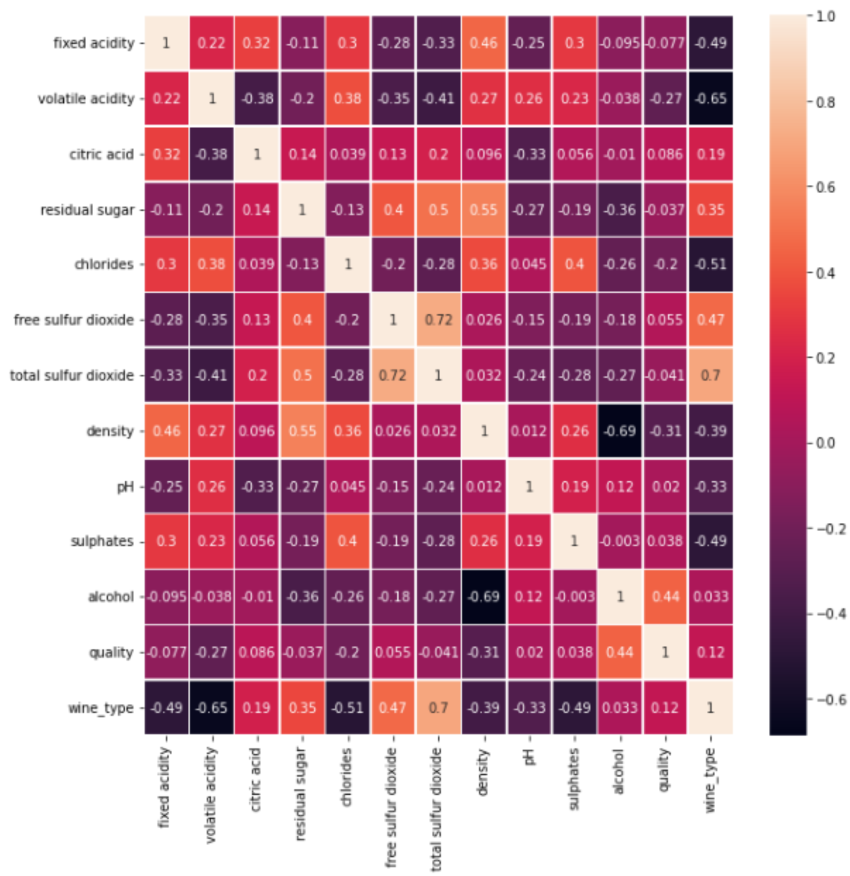
```
wine_data.hist(bins=10, figsize=(20,20))
plt.show()
```





- *Visualizing the correlation between our features:*

```
corr_matrix = wine_data.corr()
fig, ax = plt.subplots(figsize=(10,10))
sns.heatmap(corr_matrix,annot=True,linewidths=.5,ax=ax)
plt.show()
```



2) Data preprocessing

```
8] # identify highly correlated features and choose what to drop from them
for a in range(len(wine_data.corr().columns)):
    for b in range(a):
        if abs(wine_data.corr().iloc[a,b]) >0.7:
            feature = wine_data.corr().columns[a]
            print(feature)
```

```
total sulfur dioxide
```

```
# dropping features with correlation > 0.7
wine_data = wine_data.drop('total sulfur dioxide', axis=1)
wine_data.head()
```

```
wine_data.columns
```

```
Index(['fixed acidity', 'volatile acidity', 'citric acid', 'residual sugar',
       'chlorides', 'free sulfur dioxide', 'density', 'pH', 'sulphates',
       'alcohol', 'quality', 'wine_type'],
      dtype='object')
```

```
# data normalization
scaler = MinMaxScaler()
X = wine_data.drop(['wine_type'], axis=1)
X = scaler.fit_transform(X)
dataset_normalized = pd.DataFrame(X, columns=wine_data.drop(['wine_type'],axis=1).columns)
dataset_normalized['wine_type'] = wine_data['wine_type']

dataset_normalized.head()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	density	pH	sulphates	alcohol	quality	wine_type
0	0.289256	0.266667	0.192771	0.023006	0.088040	0.104167	0.196067	0.449612	0.241573	0.289855	0.666667	0
1	0.322314	0.153333	0.216867	0.056748	0.028239	0.048611	0.085020	0.302326	0.146067	0.579710	0.333333	1
2	0.214876	0.146667	0.307229	0.075153	0.064784	0.211806	0.136688	0.279070	0.129213	0.159420	0.500000	1
3	0.264463	0.226667	0.210843	0.015337	0.131229	0.052083	0.173318	0.480620	0.185393	0.173913	0.333333	0
4	0.289256	0.106667	0.204819	0.105828	0.064784	0.097222	0.175246	0.294574	0.179775	0.144928	0.333333	1

3) Train and test data preparation

```
from sklearn.model_selection import train_test_split
# our target feature is "wine_type" where 1 means white wine and 0 means red wine
dataset_classification = dataset_normalized.copy()
X = dataset_classification.drop('wine_type', axis=1)
y = dataset_classification['wine_type']
# use stratify to make sure that our target classes are balanced between train and test data
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, stratify = y)
X_train = X_train.T
y_train = np.array(y_train).reshape((1,y_train.shape[0]))
X_test = X_test.T
y_test = np.array(y_test).reshape((1,y_test.shape[0]))
```

```
[34] X_train.shape

(5197, 11)
```

```
[35] X_test.shape

(1300, 11)
```

4) Implementation and evaluation of machine learning models

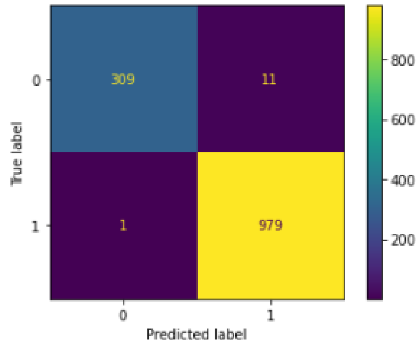
- Random forest:

```
# random forest model
rnd = RandomForestClassifier()
# fit data
fit_rnd = rnd.fit(X_train,y_train)
# predicting
y_predict = rnd.predict(X_test)

print(classification_report(y_test,y_predict))
```

```
              precision    recall  f1-score   support

           0       1.00      0.97      0.98       320
           1       0.99      1.00      0.99       980

    accuracy                           0.99      1300
   macro avg       0.99      0.98      0.99      1300
weighted avg       0.99      0.99      0.99      1300
```

```
[64] metrics.plot_confusion_matrix(rnd, X_test, y_test)
     plt.show()
```

```
/usr/local/lib/python3.8/dist-packages/sklearn/utils/deprecation.py
  warnings.warn(msg, category=FutureWarning)
```



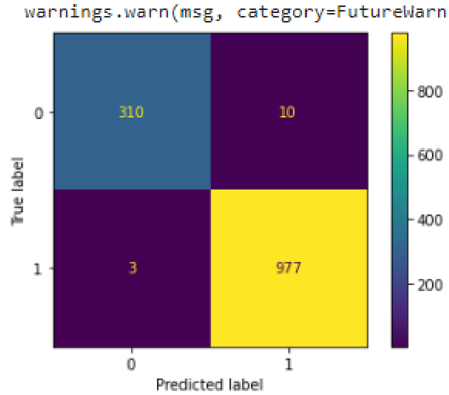
- Xgboost:

```
[62] # Xgboost model
     xgb = XGBClassifier()
     # fit data
     fit_xgb = xgb.fit(X_train,y_train)
     # predicting
     y_predict = xgb.predict(X_test)

     print(classification_report(y_test,y_predict))
```

```
              precision    recall  f1-score   support

           0       0.99      0.97      0.98       320
           1       0.99      1.00      0.99       980

    accuracy                           0.99      1300
   macro avg       0.99      0.98      0.99      1300
weighted avg       0.99      0.99      0.99      1300
```

```
metrics.plot_confusion_matrix(xgb, X_test, y_test)
plt.show()
```

```
/usr/local/lib/python3.8/dist-packages/sklearn/utils/deprecation.py
  warnings.warn(msg, category=FutureWarning)
```



5) Implementation of the neural network model

```python
# our neural network parameters initialisation
def initialisation(n0, n1, n2, n3):

  W1 = np.random.randn(n1, n0)
  b1 = np.random.randn(n1, 1)
  W2 = np.random.randn(n2, n1)
  b2 = np.random.randn(n2, 1)
  W3 = np.random.randn(n3, n2)
  b3 = np.random.randn(n3, 1)

  parameters = {
      'W1': W1,
      'b1': b1,
      'W2': W2,
      'b2': b2,
      'W3': W3,
      'b3': b3
  }

  return parameters
```

```python
[38] # implementation of the forward propagation in our neural network
def forward_propagation(X,parameters):

  W1 = parameters['W1']
  b1 = parameters['b1']
  W2 = parameters['W2']
  b2 = parameters['b2']
  W3 = parameters['W3']
  b3 = parameters['b3']

  Z1 = W1.dot(X) + b1
  A1 = 1 / (1 + np.exp(-Z1))
  Z2 = W2.dot(A1) + b2
  A2 = 1 / (1 + np.exp(-Z2))
  Z3 = W3.dot(A2) + b3
  A3 = 1 / (1 + np.exp(-Z3))

  activations = {
      'A1': A1,
      'A2': A2,
      'A3': A3
  }

  return activations
```

```python
# implementation of the backward propagation in our neural network
def back_propagation(X, y, activations, parameters):
  A1 = activations['A1']
  A2 = activations['A2']
  A3 = activations['A3']
  W2 = parameters['W2']
  W3 = parameters['W3']

  m = y.shape[1]

  dZ3 = A3 - y
  dW3 = 1 / m * dZ3.dot(A2.T)
  db3 = 1 / m * np.sum(dZ3, axis=1, keepdims=True)

  dZ2 = np.dot(W3.T, dZ3) * A2 * (1-A2)
  dW2 = 1 / m * dZ2.dot(A1.T)
  db2 = 1 / m * np.sum(dZ2, axis=1, keepdims=True)

  dZ1 = np.dot(W2.T, dZ2) * A1 * (1-A1)
  dW1 = 1 / m * dZ1.dot(X.T)
  db1 = 1 / m * np.sum(dZ1, axis=1, keepdims=True)

  gradients = {
      'dW1': dW1,
      'db1': db1,
      'dW2': dW2,
      'db2': db2,
      'dW3': dW3,
      'db3': db3
  }

  return gradients
```

```
# implementation of the parameters update in our neural network
def update(gradients, parameters, learning_rate):

  W1 = parameters['W1']
  b1 = parameters['b1']
  W2 = parameters['W2']
  b2 = parameters['b2']
  W3 = parameters['W3']
  b3 = parameters['b3']

  dW1 = gradients['dW1']
  db1 = gradients['db1']
  dW2 = gradients['dW2']
  db2 = gradients['db2']
  dW3 = gradients['dW3']
  db3 = gradients['db3']

  W1 = W1 - learning_rate * dW1
  b1 = b1 - learning_rate * db1
  W2 = W2 - learning_rate * dW2
  b2 = b2 - learning_rate * db2
  W3 = W3 - learning_rate * dW3
  b3 = b3 - learning_rate * db3

  parameters = {
      'W1': W1,
      'b1': b1,
      'W2': W2,
      'b2': b2,
      'W3': W3,
      'b3': b3
  }

  return parameters
```

```
# implementation of the target prediction in our neural network
def predict(X, parameters):
  activations = forward_propagation(X, parameters)
  A3 = activations['A3']
  predictions = []
  for i in A3[0]:
    if (i >= 0.5):
      predictions.append(1)
    else:
      predictions.append(0)
  return predictions
```

- *Now, we will implement all steps in our neural network (first hidden layer with 64 units and second hidden layer with 32units), including the calculation of the train/validation loss and train/ validation accuracy in each iteration to evaluate our model and judge if there is an overfitting or underfitting behavior. We added an early stopping callback to stop training if the validation loss doesn't decrease by more than 0.001 within 8 iterations.*

```python
def neural_network(X_train, y_train, n1, n2, learning_rate = 0.1, n_iter = 1000):

  # initialisation W, b
  n0 = X_train.shape[0]
  n3 = y_train.shape[0]
  parameters = initialisation(n0, n1, n2, n3)

  train_loss = []
  train_acc = []
  val_loss = []
  val_acc = []

  for i in range(n_iter):

    activations = forward_propagation(X_train, parameters)
    val_activations = forward_propagation(X_test, parameters)
    gradients = back_propagation(X_train, y_train, activations, parameters)
    parameters = update(gradients, parameters, learning_rate)

    # calculate train loss and accuracy
    train_loss.append(log_loss(y_train.flatten(), activations['A3'].flatten()))
    y_pred = predict(X_train, parameters)
    current_accuracy = accuracy_score(y_train.flatten(), y_pred)
    train_acc.append(current_accuracy)

    # calculate validation loss and accuracy
    val_loss.append(log_loss(y_test.flatten(), val_activations['A3'].flatten()))
    y_pred_val = predict(X_test, parameters)
    current_accuracy_val = accuracy_score(y_test.flatten(), y_pred_val)
    val_acc.append(current_accuracy_val)

    model_history = {
      'train_loss': train_loss,
      'val_loss': val_loss,
      'train_acc': train_acc,
      'val_acc': val_acc

      }
    if i != 0 and i % 8 == 0 and (val_loss[i-8]-val_loss[i]) <= 0.001 :
      print('Early stopping at ' + str(i))
      break

  return parameters, model_history
```

6) Training and evaluating the model

```
# training our model
parameters, model_history = neural_network(X_train, y_train, n1=64,n2= 32,  n_iter=1000, learning_rate=0.05)
```

```
Early stopping at 560
```

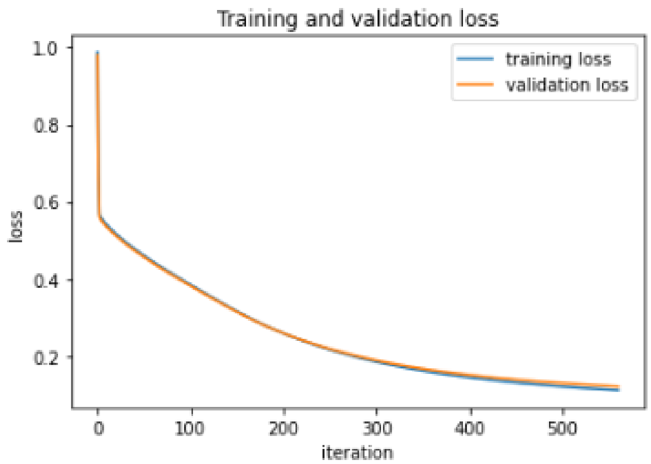
```
[97] # predicting our target validation values
y_pred_val = predict(X_test, parameters)
print(metrics.confusion_matrix(y_test.flatten(
),y_pred_val))
```

```
[[290  30]
 [ 11 969]]
```

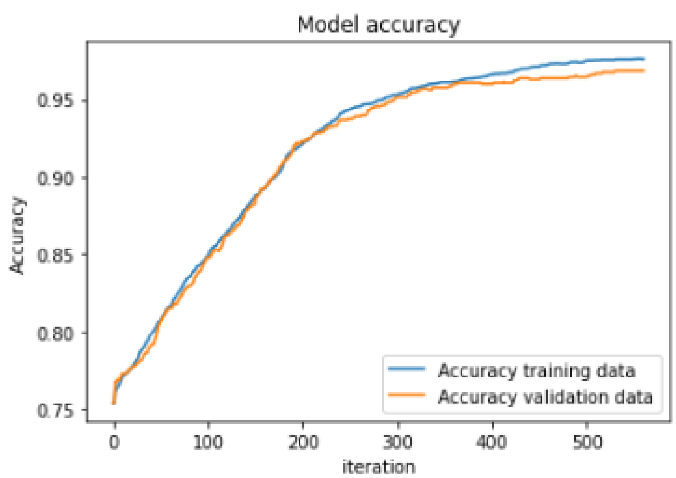
```
[98] # evaluating the model
print(classification_report(y_test.flatten(), y_pred_val))
```

```
              precision    recall  f1-score   support

           0       0.96      0.91      0.93       320
           1       0.97      0.99      0.98       980

    accuracy                           0.97      1300
   macro avg       0.97      0.95      0.96      1300
weighted avg       0.97      0.97      0.97      1300
```

```python
# the training loss indicates how well the model is fitting the training data
# while the validation loss indicates how well the model fits new data.
plt.plot(model_history['train_loss'], label='training loss')
plt.plot(model_history['val_loss'], label='validation loss')
plt.legend()
plt.title('Training and validation loss')
plt.ylabel('loss')
plt.xlabel('iteration')
plt.show()
```




```python
# plotting train and validation accuracy
plt.plot(model_history['train_acc'], label='Accuracy training data')
plt.plot(model_history['val_acc'], label='Accuracy validation data')
plt.legend()
plt.title('Model accuracy')
plt.ylabel('Accuracy')
plt.xlabel('iteration')
plt.show()
```



6) Conclusion

Our model is giving 0.97 as F1 score and there is a good fit to the train data
Some improvements could be done through:

- More data for training and testing since our classes are imbalanced
- Data augmentation
- Trying other learning rate values
- Adding neurons/layers to our architecture