Task 2 - Solution

AI4Omics Practical Session

Task 2 - Introduction to Logistic Regression

Before we start, please, execute the following code to be ready for exercises.

- Import pandas and several scikit-learn modules that will be used in the exercises:

```
[1]: import pandas as pd
     from sklearn.model_selection import train_test_split
     from sklearn import metrics
```

- Define the function `calculate_accuracy`:

```
[2]: def calculate_accuracy(classifier, X_train, X_test, y_train, y_test):
         classifier.fit(X_train, y_train)
         y_pred_train = classifier.predict(X_train)
         y_pred_test = classifier.predict(X_test)
         accuracy_train = metrics.accuracy_score(y_train, y_pred_train)
         accuracy_test = metrics.accuracy_score(y_test, y_pred_test)
         print('Train accuracy:', '{:.3f}'.format(accuracy_train), 'Test accuracy:',␣
      ↪'{:.3f}'.format(accuracy_test))
         return accuracy_train, accuracy_test, classifier
```

- Import data and create targets **y**:

```
[3]: random_state = 42
     data = pd.read_csv('../data/colon_cancer.csv', sep=';', index_col='id_sample')
     print('data', data.shape)
     y = data['tissue_status']
     print('y', y.shape)
```

```
data (804, 61)
y (804,)
```

Question 1. Create a dataframe X including all the available features (genes)

The original dataset **data** contains 60 columns with the expression levels of 60 genes and one column `tissue_status` with the sample types (normal or tumoral).

- Extract 60 columns corresponding to gene expression levels from **data** to a separate dataframe **X**.

Hint: you can use one of the methods `select_dtypes('number')` or `drop(columns=['tissue_status'])`. Please check the documentation of pandas for these two methods if you are not familiar with them.

[4]:
```
# X = data... # to complete
X = data.select_dtypes('number')
```

Question 2. Create train and test datasets with 3/4 and 1/4 of samples respectively

- Create a training dataset **X_train** and a test dataset **X_test** with their corresponding targets **y_train** and **y_test**.

[5]:
```
# X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=...,␣
↪random_state=random_state, stratify=y) # test_size to define
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=1/4,␣
↪random_state=random_state, stratify=y)
```

- How many samples contain the obtained train and test datasets?

Hint: you can use `shape` attribute of the dataframe.

[6]:
```
# print('Train:', X_train..., 'Test:', X_test...) # to complete
print('Train:', X_train.shape, 'Test:', X_test.shape)
```

```
Train: (603, 60) Test: (201, 60)
```

Question 3. Perform a standardisation of data

Data standardisation is a typical and often mandatory step in a machine learning pipeline. Data standardisation is a *feature scaling* technique aiming to convert original data, where multiple features can be spanning varying ranges and degrees of magnitude, into a comparable range of values. The data standardisation significantly improves the performance of many machine learning algorithms.

The most common standardisation technique is *Z-score* (or standard score) where the values are centered around the mean with a unit standard deviation.

Warning! The calculation of the mean μ and the standard deviation σ must be performed **on the training dataset** only. The test dataset should not be used in the calculation. It will be scaled using the values μ and σ obtained in the training dataset.

In `scikit-learn`, data standardisation can be realized with a `StandardScaler` object.

- Execute the following code to calculate μ and σ for **X_train** dataset.

[7]:
```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler() # create a scaler
```

```
scaler.fit(X_train) # calculate mu and sigma on X_train (only training dataset␣
↪should be used!)
```

```
[7]: StandardScaler()
```

- Display μ (mean) values

```
[26]: # Display calculated mu (mean) for each feature
print('Mean mu', scaler.mean_)
```

```
Mean mu [4.57607731 4.51357044 7.2181844 ]
```

- Display σ (standard deviation) values

```
[27]: # Display calculated sigma (standard deviation) for each feature
print('Std sigma', scaler.scale_)
```

```
Std sigma [1.48007846 1.61344614 1.41109107]
```

Now, we can use μ and σ calculated from **X__train** dataset to perform a standardisation of both **X__train** and **X__test**. Use the `transform` method of the `scaler`object. As a result, you should obtain two scaled datasets: **X__train__scaled** and **X__test__scaled**.

- Execute the code for **X__train**:

```
[10]: # To execute
X_train_scaled = scaler.transform(X_train) # numpy object
X_train_scaled = pd.DataFrame(X_train_scaled, index=X_train.index,␣
↪columns=X_train.columns) # convert to pandas DataFrame format
```

- Complete a similar code for **X__test** and execute it:

```
[11]: # X_test_scaled = scaler.transform(...) # to complete
X_test_scaled = scaler.transform(X_test)

# X_test_scaled = pd.DataFrame(X_test_scaled, index=...index, columns=...
↪columns) # to complete
X_test_scaled = pd.DataFrame(X_test_scaled, index=X_test.index, columns=X_test.
↪columns)
```

After the standardisation, the mean values of expression levels should be equal to 0 for all genes in **X__train__scaled**, and the standard deviation should be equal to 1.

- Check that the mean values are 0 for the first 5 features in **X__train__scaled**

```
[12]: # X_train_scaled... # to complete
X_train_scaled.mean().head()
```

```
[12]: ADH1C     7.070077e-17
DHRS11   -1.414015e-16
UGP2     -6.598739e-16
SLC7A5   -1.178346e-16
```

```
CTSS      1.089970e-16
dtype: float64
```

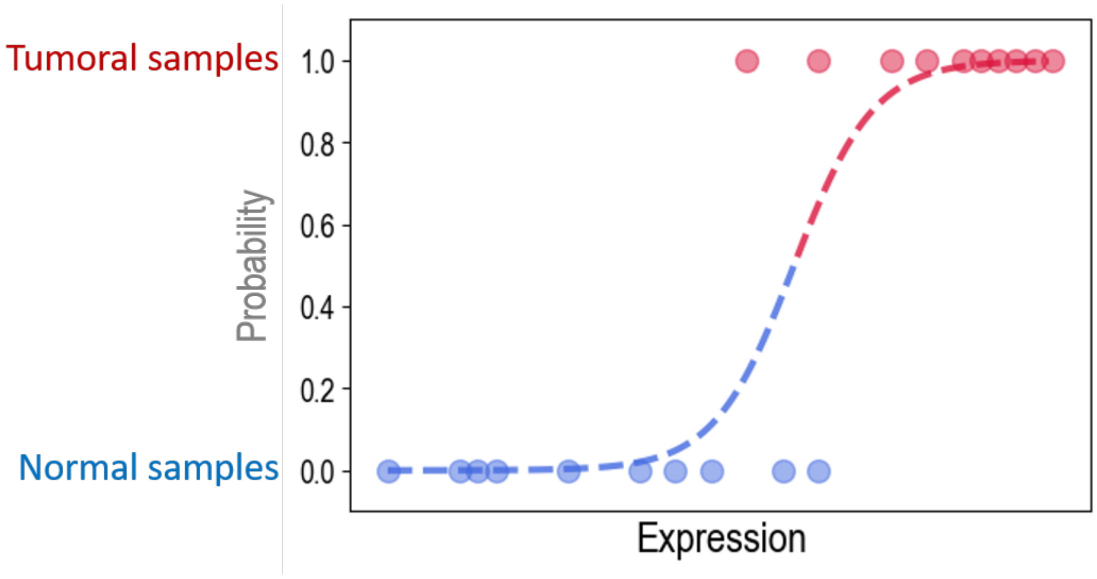
- Check that the standard deviations are 1 for the first 5 features in **X_train_scaled**

```
[13]: # X_train_scaled... # to complete
      X_train_scaled.std().head()
```

```
[13]: ADH1C     1.00083
      DHRS11    1.00083
      UGP2      1.00083
      SLC7A5    1.00083
      CTSS      1.00083
      dtype: float64
```

Question 4. Create a model of Logistic Regression (LR)

Logistic regression uses an analytical function, called *logistic function* or *sigmoid function*, which has a characteristic S-shape. By optimizing the coefficients of this function (max likelihood or min cross-entropy), it makes it possible to estimate the probability for a sample to belong to this or that class. For example, tumoral versus normal.



- Create a Logistic Regression classifier

```
[14]: from sklearn.linear_model import LogisticRegression
      classifier = LogisticRegression(random_state=random_state, penalty='none')
      print(classifier)
```

```
LogisticRegression(penalty='none', random_state=42)
```

- Train the classifier and calculate its accuracy using `calculate_accuracy` function

```
[15]: # accuracy_train, accuracy_test, trained_classifier =␣
       ↪calculate_accuracy(classifier, ... , ... , y_train, y_test) # to complete
      accuracy_train, accuracy_test, trained_classifier =␣
       ↪calculate_accuracy(classifier, X_train_scaled, X_test_scaled, y_train,␣
       ↪y_test)
```

```
Train accuracy: 1.000 Test accuracy: 1.000
```

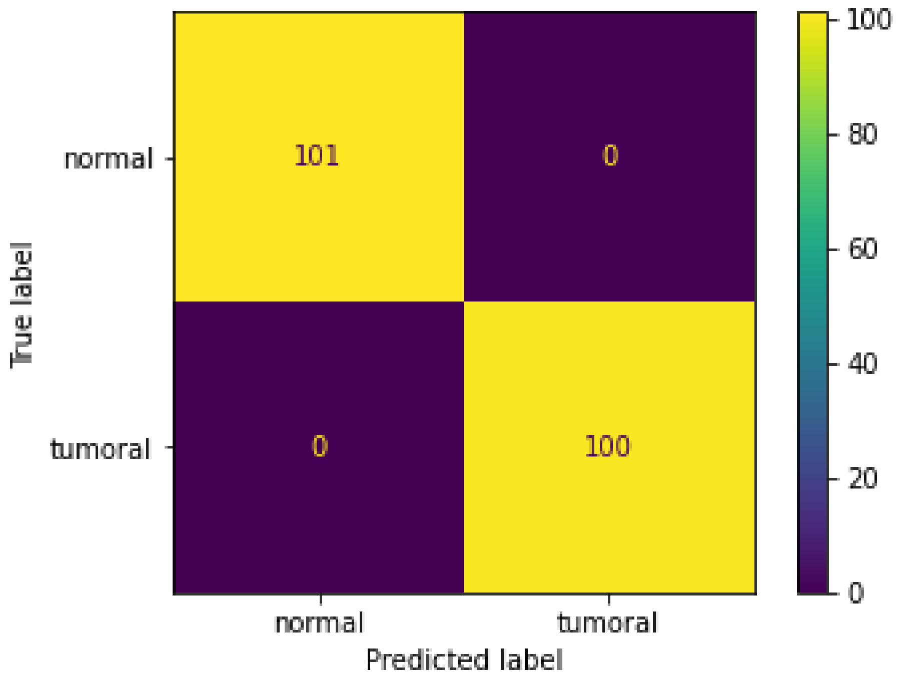
Question 5. Display a confusion matrix for LR algorithm

A *confusion matrix* is a table that allows visualisation of the performance of a supervised algorithm. Each row of the matrix represents the instances in an actual class while each column represents the instances in a predicted class.

- Display a confusion maxtrix for LR algorithm **using the test dataset only**

```
[16]: # metrics.plot_confusion_matrix(trained_classifier, ... , ...) # to complete
      metrics.plot_confusion_matrix(trained_classifier, X_test_scaled, y_test)
```

```
[16]: <sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1a6ebdbcc70>
```



Question 6. Evaluate the impact of each gene in LR classifier

After the training phase, it is possible to know the coefficients β of LR model for each feature (gene). They are available in the `coef_` attribute. The greater is the coefficient β (in absolute value), the greater is the impact of the corresponding gene in the model. By analysing the coefficients β of the trained LR model, we can find the most predictive genes.

- Display the coefficients β for the first 5 features.

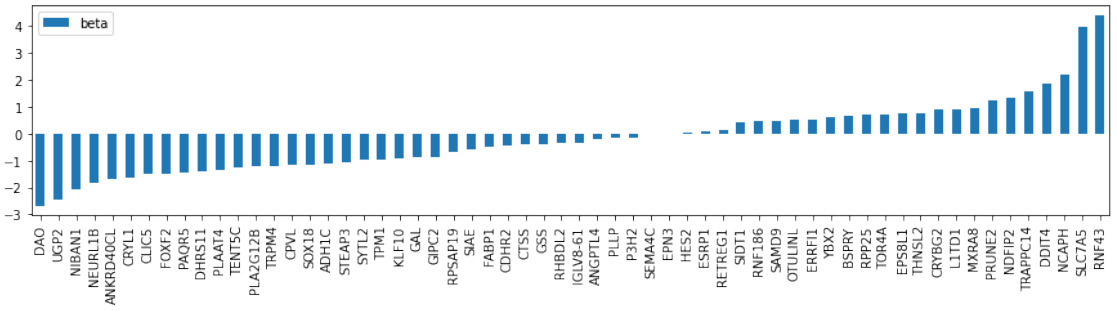
```
[17]: coefficients = pd.DataFrame(trained_classifier.coef_[0], index=X_train_scaled.
       ↪columns, columns=['beta'])
      coefficients.head()
```

```
[17]:             beta
      ADH1C  -1.095463
      DHRS11 -1.412367
      UGP2   -2.444311
      SLC7A5  3.980374
      CTSS   -0.411723
```

- Display the coefficients β as a *barplot* from the smallest to the biggest value.

```
[18]: coefficients = coefficients.sort_values(by='beta')
      coefficients.plot.bar(figsize=(15, 3))
```

```
[18]: <AxesSubplot:>
```



- What genes have the most important impact in the model?
- What genes have almost no impact on the prediction?
- Select the best 3 features mostly impacting the model

```
[19]: n_features = 3
      coefficients['abs_beta'] = coefficients['beta'].abs() # calculate the absolute␣
       ↪values of betas
      coefficients = coefficients.sort_values(by='abs_beta', ascending=False) # sort␣
       ↪by arsolute values
      top_features = list(coefficients.head(n_features).index) # list of N top␣
       ↪features
      print('Top features of LR:', top_features)
```

```
Top features of LR: ['RNF43', 'SLC7A5', 'DAO']
```

Question 7. Calculate the performace of LR model using 1, 2, ... N top features

- What does the code below calculate? Execute it and explain the result.

```
[20]: for i in range(len(top_features)):
          selected_features = top_features[0:i+1]
          print(selected_features)
          accuracy_train, accuracy_test, trained_classifier =␣
       ↪calculate_accuracy(classifier, X_train_scaled[selected_features],␣
       ↪X_test_scaled[selected_features], y_train, y_test)
```

```
['RNF43']
Train accuracy: 0.919 Test accuracy: 0.841
['RNF43', 'SLC7A5']
Train accuracy: 0.964 Test accuracy: 0.935
['RNF43', 'SLC7A5', 'DAO']
Train accuracy: 0.992 Test accuracy: 0.990
```

- Do we need all the 60 genes in the model? What do you think? If we can reduce the number of features, how many should we keep?

Question 8. Case study

The *AI-Hospital* has developed a new diagnostic tool for colon cancer based on the expression levels of a panel of 3 genes. This tool produced the following measurements for a new patient arrived in the hospital:

```
[21]: panel = ['RNF43', 'SLC7A5', 'DAO']
```

```
[22]: new_patient = {'RNF43': 4.68, 'SLC7A5': 4.10, 'DAO': 7.59}
```

- **Does this patient have a colon cancer?**

Hint: To answer this question, train a LR model on the totality of available data **X**. In this case, **X__train** will contain all the samples of **X**. **X__test** will have only one sample corresponding to the new patient. Do not forget to scale the data properly, `fit` on **X__train** only and then `transform` on both **X__train** and **X__test**.

```
[23]: X_train = data[panel]
      y_train = y
      X_train.head(3)
```

```
[23]:                    RNF43    SLC7A5       DAO
      id_sample
      EPSM-COLON-0001  4.241267  3.864253  8.465133
      EPSM-COLON-0002  4.002000  3.069581  8.159814
      EPSM-COLON-0003  3.447174  3.188257  8.004194
```

```
[24]: X_test = pd.DataFrame([new_patient], index=['new_patient'])
      X_test
```

```
[24]:               RNF43  SLC7A5   DAO
      new_patient    4.68     4.1  7.59
```

```
[25]: # Code to write by yourself

      scaler = StandardScaler()
      scaler.fit(X_train)
      X_train_scaled = scaler.transform(X_train)
      X_test_scaled = scaler.transform(X_test)

      classifier = LogisticRegression(random_state=random_state, penalty='none')
      classifier.fit(X_train_scaled, y_train)
      y_new_patient = classifier.predict(X_test_scaled)
      print(classifier, y_new_patient)
```

```
LogisticRegression(penalty='none', random_state=42) ['normal']
```