task2_solution

July 18, 2023

1 AI4Omics Practical Session

1.1 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,)
```

1.2 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')
```

1.3 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)
```

1.4 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

[8]:
```
# Display calculated mu (mean) for each feature
print('Mean mu', scaler.mean_)
```

```
Mean mu [5.56250784 4.37031229 5.5576452  4.5032885  6.70477296 7.20224541
 2.73722189 2.83883913 3.09567408 3.62783178 4.9956429  8.00645284
 2.13428824 3.25051517 5.72798593 2.602014   5.09621073 4.95027125
 5.12856168 2.60945896 4.57087133 2.61901627 4.00316847 2.83774532
 5.05378073 4.70302486 4.48579809 5.2552879  5.10330709 3.87416991
 4.42493323 3.41604512 2.99677417 3.12825274 3.21237453 2.94096313
 4.059025   2.56226458 4.03283796 2.46987601 3.61611895 3.06480367
 4.18373897 3.33961906 4.60751801 3.22049712 4.79100352 3.19601853
 2.16639761 5.46168857 3.59541576 4.6518569  4.25604076 4.60405964
 4.10572903 1.79212905 2.84821267 6.10344378 2.81507307 2.61131882]
```

- Display σ (standard deviation) values

[9]:
```
# Display calculated sigma (standard deviation) for each feature
print('Std sigma', scaler.scale_)
```

```
Std sigma [2.87450773 1.41750502 1.16900926 1.62727559 1.08192036 1.39528512
 1.4405307  1.25002277 1.20996386 1.2651503  0.7258847  3.02651441
 0.6970907  0.8496204  1.10564825 1.29408208 1.25535892 2.70235274
 0.83604128 1.45557859 1.36504482 0.89653108 0.89616633 0.74177497
 0.76354578 1.08303667 0.89196864 1.07683176 1.1278559  0.959783
 0.94799683 0.95342434 0.95399801 1.05874883 0.91663639 0.79398048
 0.86882235 0.95497763 0.74386269 0.79827373 0.58288541 1.14404363
 0.75023715 0.78168341 1.51741848 0.91180632 1.10693458 1.12902104
 0.83743434 1.17059202 1.06519408 0.93742726 1.65998753 0.86348611
 1.26049718 0.70875365 1.33154111 0.84309529 1.02498105 0.99669006]
```

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
```

1.5 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
```

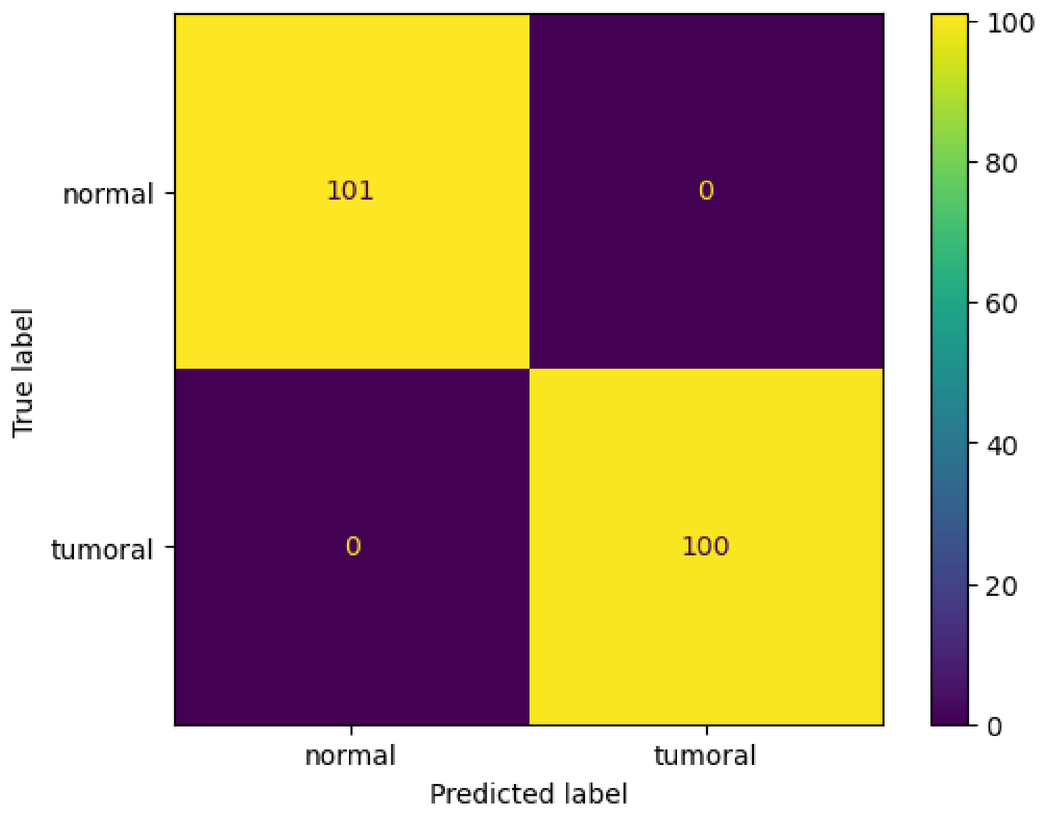
1.6 Question 5. Display a confusion matrix for LR algorithm

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]:
```
from sklearn.metrics import ConfusionMatrixDisplay
# ConfusionMatrixDisplay.from_estimator(trained_classifier, ..., ...) # to␣
 ↪complete
ConfusionMatrixDisplay.from_estimator(trained_classifier, X_test_scaled, y_test)
```

[16]:
```
<sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x23b1eea0640>
```



1.7 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.

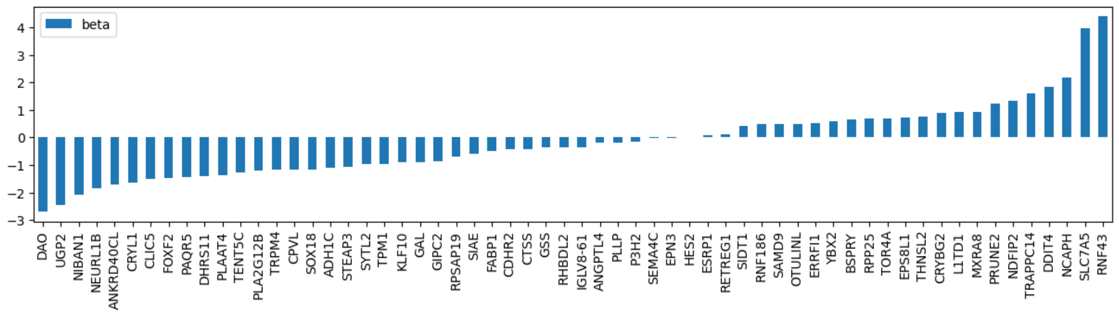
```
[17]: coefficients = pd.DataFrame(trained_classifier.coef_[0], index=X_train_scaled.
        ↪columns, columns=['beta'])
      coefficients.head()
```

```
[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]: <Axes: >
```



- 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']
```

1.8 Question 7. Calculate the performance 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?

1.9 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]:
```python
X_test = pd.DataFrame([new_patient], index=['new_patient'])
X_test
```

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

[25]:
```python
# 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']
```

[ ]:
```python
```