# task1_solution

July 18, 2023

## 1 AI4Omics Practical Session

### 1.1 Task 1 - Introduction to classification models in machine learning

### 1.2 1. Import data

Import `pandas` package which allows us to perform data analysis and manipulation of dataframes in Python.

[1]:
```
import pandas as pd
```

The data are available in the file `colon_cancer.csv`. Data import is done with the pandas `read_csv` command. The `shape` attribute contains the dimensions of the dataframe.

[2]:
```
data = pd.read_csv('../data/colon_cancer.csv', sep=';', index_col='id_sample')
print('data', data.shape)
```

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

The `head()` method displays by default the first 5 lines of the dataframe. If necessary, we can indicate the number of lines to display, for example `head(3)` for 3 lines.

[3]:
```
data.head()
```

[3]:

| id_sample | ADH1C | DHRS11 | UGP2 | SLC7A5 | CTSS | DAO | \ |
|---|---|---|---|---|---|---|---|
| EPSM-COLON-0001 | 9.199944 | 6.090054 | 7.062512 | 3.864253 | 7.869368 | 8.465133 | |
| EPSM-COLON-0002 | 7.767618 | 6.027985 | 6.318818 | 3.069581 | 6.410334 | 8.159814 | |
| EPSM-COLON-0003 | 7.918904 | 5.885948 | 6.917742 | 3.188257 | 7.915549 | 8.004194 | |
| EPSM-COLON-0004 | 9.053553 | 6.027985 | 7.081085 | 2.357523 | 5.657726 | 8.004194 | |
| EPSM-COLON-0005 | 6.027822 | 5.791257 | 5.937685 | 4.137667 | 5.818999 | 8.056067 | |

| id_sample | NIBAN1 | PRUNE2 | FOXF2 | TENT5C | … | BSPRY | \ |
|---|---|---|---|---|---|---|---|
| EPSM-COLON-0001 | 1.174665 | 0.975086 | 3.028995 | 6.350919 | … | 5.528372 | |
| EPSM-COLON-0002 | 5.959414 | 1.625518 | 2.984629 | 4.686086 | … | 5.671788 | |
| EPSM-COLON-0003 | 1.560386 | 2.379909 | 2.929762 | 4.281126 | … | 4.596079 | |
| EPSM-COLON-0004 | 3.548988 | 3.260031 | 3.313829 | 4.821072 | … | 4.135061 | |
| EPSM-COLON-0005 | 3.307945 | 5.208874 | 4.191695 | 5.181036 | … | 3.674043 | |

```
                    CDHR2    ERRFI1     CLIC5      PLLP       GAL     CRYL1  \
id_sample
EPSM-COLON-0001  3.500730  2.893760  5.130743  1.485110  1.830484  6.379933
EPSM-COLON-0002  4.658790  4.715374  5.438104  2.131466  2.097157  6.863173
EPSM-COLON-0003  5.649376  4.047899  6.580938  1.447209  3.890943  6.209704
EPSM-COLON-0004  5.437107  4.537381  4.615263  1.004454  1.840902  6.774063
EPSM-COLON-0005  6.286182  4.715374  4.432410  0.159195  3.506561  6.150297

                     YBX2   ANGPTL4  tissue_status
id_sample
EPSM-COLON-0001  3.919293  3.031413         normal
EPSM-COLON-0002  0.322829  3.978531         normal
EPSM-COLON-0003  3.274407  3.714491         normal
EPSM-COLON-0004  3.320525  3.080796         normal
EPSM-COLON-0005  0.461184  5.140305         normal

[5 rows x 61 columns]
```

The data contain the expression levels of **60 genes** in **804 samples** of colon tissue. The last column `tissue_status` indicates if the sample is normal or tumoral.

The data types of each column can be displayed with `dtypes`.

[4]:
```
data.dtypes
```

[4]:
```
ADH1C            float64
DHRS11           float64
UGP2             float64
SLC7A5           float64
CTSS             float64
                  …
GAL              float64
CRYL1            float64
YBX2             float64
ANGPTL4          float64
tissue_status     object
Length: 61, dtype: object
```

We can see that the data are mostly *float values* except for `tissue_status` which is actually a *string*, considered as an *object* by pandas.

The `describe` method displays descriptive statistics of numerical data only. The `tissue_status` column will not be included.

[5]:
```
data.describe()
```

[5]:
```
             ADH1C      DHRS11        UGP2      SLC7A5        CTSS         DAO  \
count  804.000000  804.000000  804.000000  804.000000  804.000000  804.000000
mean     5.588943    4.354817    5.557694    4.513570    6.717535    7.218184
```

```
std      2.889901    1.431179    1.150565    1.614450    1.077821    1.411969
min      0.610504    1.427079    2.027201    1.685024    3.668691    1.164886
25%      3.174250    3.118844    4.611060    3.030022    6.065937    6.241714
50%      5.467024    4.125990    5.412204    4.382953    6.762908    7.578782
75%      8.444756    5.696566    6.556969    5.918848    7.485487    8.263561
max     10.263846    7.022241    7.571114    8.059430    8.990703   10.079135

           NIBAN1      PRUNE2       FOXF2      TENT5C  …       SYTL2  \
count  804.000000  804.000000  804.000000  804.000000  …  804.000000
mean     2.737937    2.806573    3.064394    3.658318  …    3.599294
std      1.466906    1.243826    1.191486    1.258059  …    1.054504
min      0.716737    0.368200    0.610504    0.858074  …    1.286220
25%      1.550382    1.864561    2.198244    2.655091  …    2.878356
50%      2.297732    2.741509    2.900393    3.605686  …    3.613342
75%      3.669509    3.574304    3.752899    4.686086  …    4.417632
max      6.682541    6.591924    6.276628    6.350919  …    5.713776

           BSPRY       CDHR2      ERRFI1       CLIC5        PLLP         GAL  \
count  804.000000  804.000000  804.000000  804.000000  804.000000  804.000000
mean     4.682718    4.225014    4.575397    4.097244    1.823268    2.822931
std      0.917027    1.656088    0.859138    1.276589    0.721587    1.338349
min      1.868389    0.637047    2.250347    1.015235    0.118945    0.610504
25%      4.349295    2.921069    3.958903    3.131267    1.337715    1.840902
50%      4.869313    4.116251    4.537381    3.975276    1.689671    2.591044
75%      5.249372    5.507864    5.070072    5.118110    2.211967    3.661012
max      7.029946    9.045672    7.647284    7.129499    4.763212    7.545757

           CRYL1        YBX2     ANGPTL4
count  804.000000  804.000000  804.000000
mean     6.096634    2.801603    2.596452
std      0.840122    1.011971    1.000962
min      2.031471    0.000000    0.757246
25%      5.489589    2.277491    1.824823
50%      6.150297    2.905605    2.442378
75%      6.728052    3.505721    3.139738
max      8.723941    5.169059    6.493643

[8 rows x 60 columns]
```

### 1.3 2. Display distributions of expression levels

To create graphical plots we will use the graphical packages of Python `matplotlib` and `seaborn`.

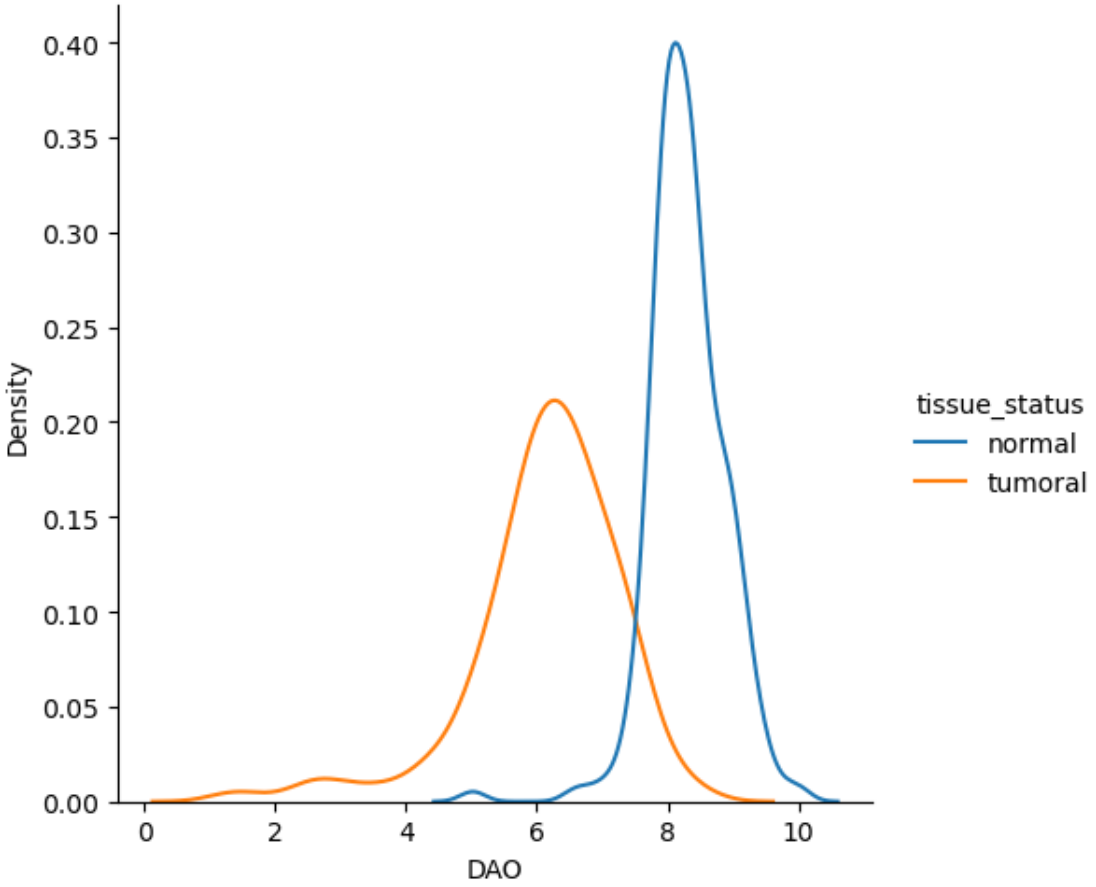
[6]:
```
%matplotlib inline
import seaborn as sns
import matplotlib.pyplot as plt
```

The `displot` command of the `seaborn` package enables us to display a distribution of values (as a

kernel density estimator *kde* or as a histogram *hist*). Let's select one gene, for example *DAO*, and plot the distribution of expression levels of this gene across all samples.

[7]:
```
selected_gene = 'DAO'
sns.displot(data=data, x=selected_gene, hue='tissue_status', kind='kde')
```

[7]: <seaborn.axisgrid.FacetGrid at 0x2b510cbea00>




The gene *DAO* is highly expressed in normal samples while its expression in tumour samples is much lower.

We can intuitively feel that if we introduce a certain threshold for *DAO* expression, for example 7.5, we will be able to predict for any new sample if it is normal or tumoral. For this, we just need to measure the level of *DAO* expression in the new sample. If it is below 7.5 than the sample is tumoral, otherwise it is normal.

### 1.4 3. Create features and targets for machine learning

For machine learning purposes in Python, we usually prepare data in two separate objects: - The first object is a matrix (or a dataframe) of *data*, typically named **X**, which contains the

measurements for all available variables (features). In our case, the features are the 60 genes. The dataframe **X** contains the expression levels of these genes (features). - The second object is a list of *targets* that we aim to predict, named **y**. In our example, it corresponds to the column `tissue_status` containing the types of each sample, normal tissue or cancer.

Let's consider a simple case when we have only one gene *DAO*. What would be the data **X** and the targets **y**?

In this case, we have only one feature, the gene *DAO*. The dataframe **X** will therefore contain the expression levels of this gene in all the samples.

[8]:
```
features = ['DAO']
X = data[features] # dataframe (pandas)
X.head(3)
```

[8]:

| | DAO |
|---|---|
| id_sample | |
| EPSM-COLON-0001 | 8.465133 |
| EPSM-COLON-0002 | 8.159814 |
| EPSM-COLON-0003 | 8.004194 |

The targets **y** correspond to the column `tissue_status` containing the types of each sample. It can be implemented as a *list* in Python or a *numpy.array* or a *pandas.Series*. We will use the last option.

[9]:
```
y = data['tissue_status'] # series (pandas)
print(y)
```

```
id_sample
EPSM-COLON-0001     normal
EPSM-COLON-0002     normal
EPSM-COLON-0003     normal
EPSM-COLON-0004     normal
EPSM-COLON-0005     normal
                    …
EPSM-COLON-0800    tumoral
EPSM-COLON-0801    tumoral
EPSM-COLON-0802    tumoral
EPSM-COLON-0803    tumoral
EPSM-COLON-0804    tumoral
Name: tissue_status, Length: 804, dtype: object
```

### 1.5 4. Create training and test datasets

In a machine learning approach, it is mandatory to split the initial dataset **X** into two datatsets: one dataset **X_train** will be used to train the model and the other **X_test** to test its efficiency. The samples for these datasets will be selected randomly.

To create the datasets **X_train** and **X_test**, we will use the framework `scikit-learn` which contains a dedicated tool `train_test_split`.

[10]:
```
from sklearn.model_selection import train_test_split
```

Let's use 2/3 of samples from the original dataset **X** as a training set **X__train**, and another 1/3 of samples as a test set **X__test**.

[11]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=1/3,␣
 ↪random_state=42, stratify=y)
print('Train dataset:', X_train.shape, 'Test dataset:', X_test.shape)
```

```
Train dataset: (536, 1) Test dataset: (268, 1)
```

We automatically generated **X__train** and **X__test** datasets with their corresponding targets **y__train** and **y__test**.

The option `random_state` in `train_test_split` initializes a random generator. The option `stratify` indicates that the proportions of tumour and normal samples in both **X__train** and **X__test** datasets should be the same as in the initial dataset **X** (50/50 in our case).

Now, if we display the samples included in the training dataset **X__train**, we can see that the initial samples have been shuffled and randomly selected. The order of samples from the original dataset **X** is not conserved.

[12]:
```
X_train.head(3)
```

[12]:

| id_sample | DAO |
|---|---|
| EPSM-COLON-0782 | 5.458151 |
| EPSM-COLON-0754 | 6.173560 |
| EPSM-COLON-0577 | 6.870016 |

Same for **X__test**.

[13]:
```
X_test.head(3)
```

[13]:

| id_sample | DAO |
|---|---|
| EPSM-COLON-0691 | 6.543940 |
| EPSM-COLON-0435 | 7.598907 |
| EPSM-COLON-0508 | 4.271774 |

### 1.6 5. Training a Decision Tree

A decision tree during the training step search for an optimal threshold that allows to separate normal and tumour samples. The `max_depth` option indicates the maximum depth of the tree. The `fit` method performs the training of the model. The training of the model is done only on the training dataset **X__train**.

[14]:
```
from sklearn.tree import DecisionTreeClassifier
classifier = DecisionTreeClassifier(max_depth=1, random_state=42,␣
 ↪criterion='entropy')
classifier.fit(X_train, y_train)
```

[14]:
```
DecisionTreeClassifier(criterion='entropy', max_depth=1, random_state=42)
```

It could be interesting to display the optimal threshold found by the algorithm during the learning process. We can do it with the `export_text` function.

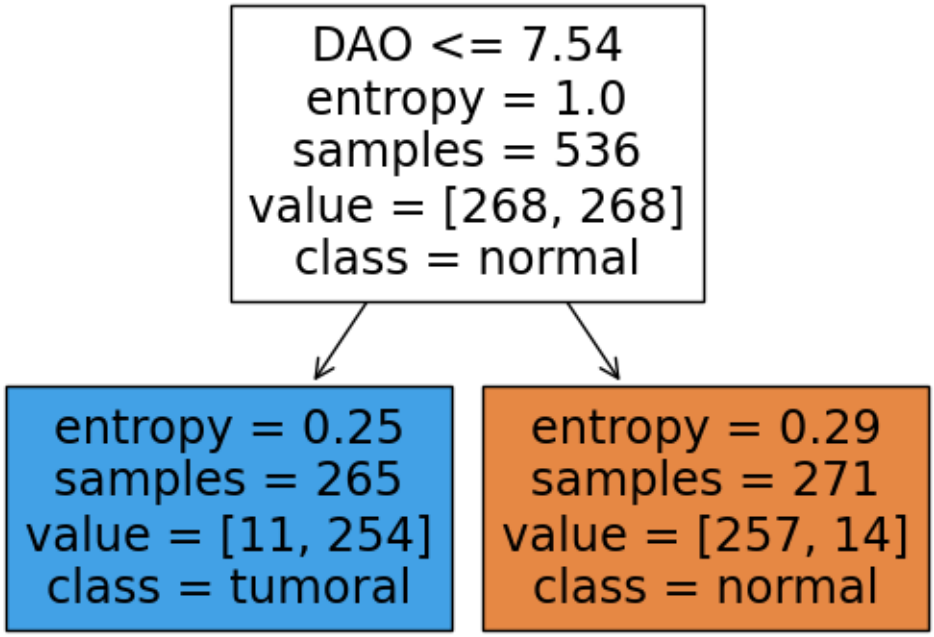
[15]:
```
from sklearn.tree import export_text, plot_tree
decision_tree_text = export_text(classifier, feature_names=list(X_train.
  ↪columns))
print(decision_tree_text)
```

```
|--- DAO <= 7.54
|   |--- class: tumoral
|--- DAO >  7.54
|   |--- class: normal
```

We can also visualize the obtained decision tree when it is not too complex. The `plot_tree` function generates the graph.

[16]:
```
plot_tree(classifier, feature_names=list(X_train.columns),  class_names=y.
  ↪unique(), precision=2, filled=True)
```

[16]:
```
[Text(0.5, 0.75, 'DAO <= 7.54\nentropy = 1.0\nsamples = 536\nvalue = [268,
268]\nclass = normal'),
 Text(0.25, 0.25, 'entropy = 0.25\nsamples = 265\nvalue = [11, 254]\nclass =
tumoral'),
 Text(0.75, 0.25, 'entropy = 0.29\nsamples = 271\nvalue = [257, 14]\nclass =
normal')]
```




### 1.7 6. Predict the diagnosis of new patients (test dataset)

Once the model has been trained, it can be used on new samples to predict their status (normal or tumour). The performance of the model is usually estimated by a metric. In our example, we will use the *accuracy* metric.

**Accuracy** = Number of correct predictions / Total number of predictions

The prediction can be done with the `predict` method. In `scikit-learn`, all the supervised machine learning models have at leat two standard methods: `fit` to train the model (on train dataset) and `predict` to perform a prediction (on test dataset).

[17]:
```
y_pred_train = classifier.predict(X_train)
y_pred_test = classifier.predict(X_test)
```

The accuracy calculation is available in `metrics` module of `scikit-learn`.

[18]:
```
from sklearn import metrics
accuracy_train = metrics.accuracy_score(y_train, y_pred_train)
accuracy_test = metrics.accuracy_score(y_test, y_pred_test)
print('Train accuracy:', '{:.2f}'.format(accuracy_train), 'Test accuracy:', '{:.
  ↪2f}'.format(accuracy_test))
```

```
Train accuracy: 0.95 Test accuracy: 0.93
```

To **evaluate a model**, we essentially take into account the **metric calculated on the test**

**dataset**. Sometimes, we can also compare it with the metric obtained on the training dataset to know if the model tends to overfit.

### 1.8 7. Create a function that performs all steps

Subsequently, in the following exercises we will often perform the training, prediction and metric calculation steps for different machine learning models. It will be more convenient for us to create a special `calculate_accuracy` function that performs all these steps automatically.

[19]:
```
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:', '{:.2f}'.format(accuracy_train), 'Test accuracy:',␣
 ↪'{:.2f}'.format(accuracy_test))
    return accuracy_train, accuracy_test, classifier
```

Example of use:

[20]:
```
accuracy_train, accuracy_test, trained_classifier =␣
 ↪calculate_accuracy(classifier, X_train, X_test, y_train, y_test)
```

```
Train accuracy: 0.95 Test accuracy: 0.93
```

*Disclaimer! The function* `calculate_accuracy` *is proposed here to simplify the code of the lesson, for teaching purposes only. In this example, it is convenient for us to add all the steps in the same function. Nevertheless, if you need to produce a professional code for production purposes, please take into account good practices of software engineering. Usually, the good practices recommend to separate different actions in different atomic functions and don't mix the calculation and the presentation of data/results. A concrete approach may depend on the programming paradigm.*

**Congratulations, you successfully completed the task 1! Please, proceed to the task 2.**