T-Lymphocytes Classification

Miradain Atontsa (miradain.atontsan@gmail.com)

August 14, 2020

The goal of this report is to use Machine Learning algorithms to classify the T-Lymphocytes in two groups: T-helper and T-regulatory. To answer to this classification problem, we will follow the classical machine learning framework:

- Exploratory data analysis;
- Feature selection;
- Model selection along with performance assessment;
- Choosing the most suitable algorithm.

1 Loading the data

```
# Import the libraries
import pandas as pd
import numpy as np
from pandas import read_csv

# Loading the training data
train_df = read_csv("/Users/miradain/Desktop/Machine_Learning_Q2/
 ↪ML-A5-2020_train.csv", index_col=0)
```

2 Exploratory data analysis

- Getting the infos on the data

```
train_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 1000 entries, C-1 to C-1000
Columns: 23385 entries, A1BG to label
dtypes: bool(8), float64(23371), int64(2), object(4)
memory usage: 178.4+ MB
```

The data has 1000 users and 23385 features: 8 boolean features, 23371 numerical features, 4 categorical features and 2 integer features (among those, there is the dependent variable 'label').

- Checking the group proportions in the dependant variable

```
train_df['label'].astype(str).value_counts()
```

```
-1    885
1     115
Name: label, dtype: int64
```

We deduce that the data is unbalanced as there are a disproportionate ratio of observations in each class: 11.5% T-reg (+1) and 88.5% T-helper (-1). This suggest that a "majority vote" strategy can even do better than a sophisticated model if we use a naive metric. This kind of problem often occurs in machine learning classification and there are many ideas to solve it. Our approach will consist of changing evaluation the metric. Namely, we will consider a weighted average between the sensitivity and the specificity.

- Building the performance evaluation metric

The metric that we use in this report is the Balanced Classification Rate (BCR) which considers sensitivity and speficity similarly:

$$BCR = \frac{1}{2}\left(\frac{TP}{TP+FN} + \frac{TN}{TN+FP}\right)$$

The above cited "majority vote" will give a score BCR $= 0.5$.

```
from sklearn.metrics import  make_scorer
from sklearn.metrics import confusion_matrix

def BCR_fun(y_true, y_pred):
    Table_Pred_BCR = confusion_matrix(y_true, y_pred)
    n1 = Table_Pred_BCR[0,0]+Table_Pred_BCR[1,0]
    n2 = Table_Pred_BCR[1,1]+Table_Pred_BCR[0,1]
    speficity_pred = Table_Pred_BCR[0,0]/(max(n1,1))
    sensitivity_pred = Table_Pred_BCR[1,1]/(max(n2,1))
    return 1/2*(speficity_pred + sensitivity_pred)

BCR_score = make_scorer(BCR_fun, greater_is_better=False)
```

- Checking the proportion of missing data

```
sum(train_df.isna().sum())/(23371*1000)
```

```
0.03493072611355954
```

Thus the data has $\sim$ 3.5% of missing data.

- Filling the missing values of numerical features with their respective median

```
# Extract the float64 and int64 part of the data
```

```
num_train_df= train_df.loc[:,(train_df.dtypes==np.float64) | (train_df.
 ↪dtypes==np.int64)]

X=train_df.fillna(num_train_df.median()).drop('label', axis=1)
y=train_df['label']
```

3 Feature selection

The data has too many features and this step aims to select (univariate selection) only those which are "significant" to the dependent variable. More concretely, we will select the 1000 features with the highest score on the test chi-squared statistic with the dependent variable. For the numerical variables, we will first remove features with low variance as these don't affect the prediction. So removing them will reduce the computation time.

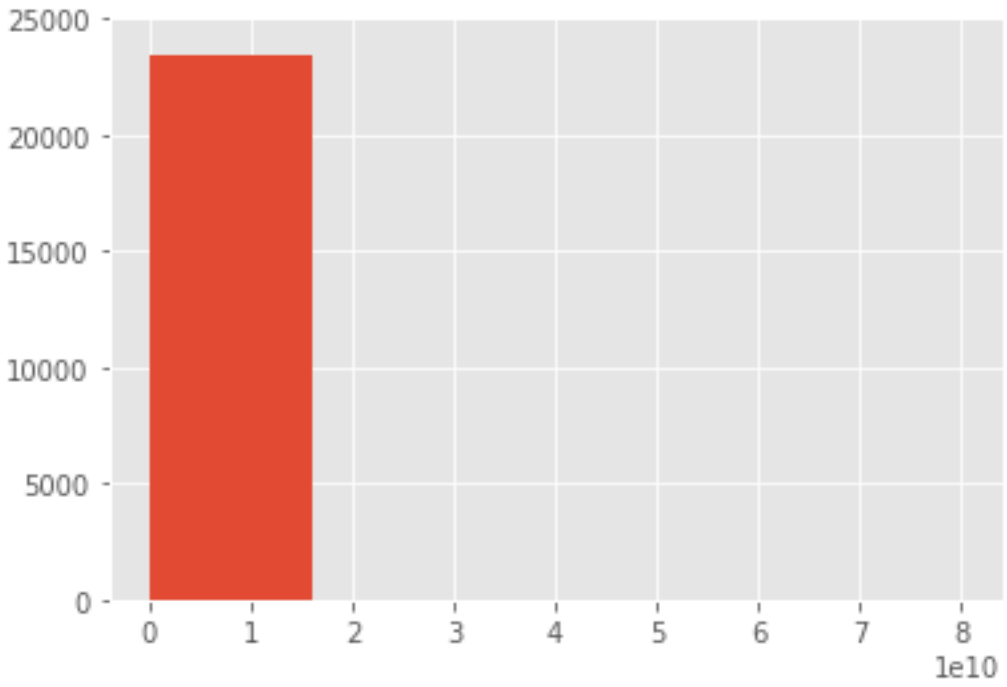
3.1 Numerical feature selection

- Removing numerical features with low variance

```
# Extract numerical and integer features
X_num_int= X.loc[:, (X.dtypes==np.float64) | (X.dtypes==np.int64)]
Covariance_matrix=X_num_int.cov()
variances= pd.DataFrame( np.diag(Covariance_matrix), index= Covariance_matrix.
 ↪index, columns= ['variance'])
```

Before extracting the high variance features, we will make a visualisation to decide about the treshold.

```
import matplotlib.pyplot as plt
plt.style.use('ggplot')
plt.hist(np.array(variances), 5)
plt.ylim(bottom=0, top= 25000)
plt.show()
```



We will consider features with variance above 7000. They are 5784.

```
Var= variances[variances.variance>=7000]
len(Var)
Numerical_Features=Var.index.values.tolist()
```

- We use the ch2 method to select useful numerical features

```
from sklearn.feature_selection import SelectKBest, chi2
import matplotlib.pyplot as plt

fs=SelectKBest(score_func=chi2, k=988)
fs.fit(X[Numerical_Features], y)
index= fs.get_support(indices=True)
Num_Features=[Numerical_Features[i] for i in index]
```

3.2 Categorical feature selection

- We encode categorical (object) features into numerical ones.

patient: 'Alpha'=0, 'Beta'=1, 'Gamma'= 2, 'Delta'=3, 'Epsilon'=4

tissue: 'Periferal blood'=0, 'Tumor-infiltrating'=1, 'Normal'=2

level.mito: 'High'=0, 'Normal'=1

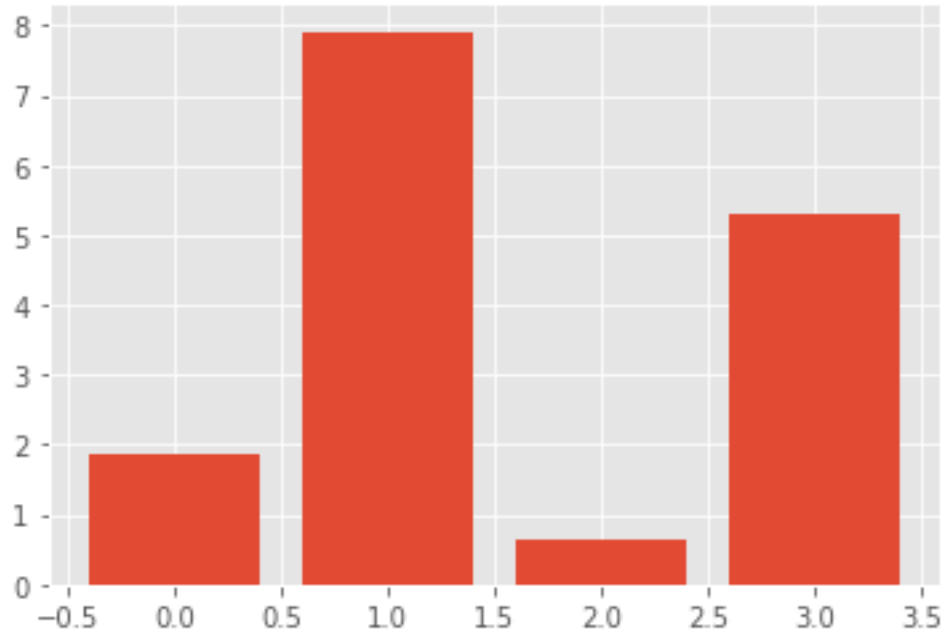
level.ribo: 'High'=0, 'Normal'=1

```
X['patient'], uniques_patient=pd.factorize(X['patient'])
X['tissue'], uniques_tissue=pd.factorize(X['tissue'])
X['level.mito'], uniques_level_mito=pd.factorize(X['level.mito'])
X['level.ribo'], uniques_level_ribo=pd.factorize(X['level.ribo'])
```

- We use the ch2 method to select useful categorical variables

```
cat_features=['patient', 'tissue', 'level.mito', 'level.ribo']
X_catt=X[cat_features]

from sklearn.feature_selection import SelectKBest, chi2
import matplotlib.pyplot as plt

fs=SelectKBest(score_func=chi2, k='all')
fs.fit(X_catt, y)

for i in range(len(fs.scores_)):
    print('Feature %d: %f' %(i, fs.scores_[i]))

# Plot the scores
plt.bar([i for i in range(len(fs.scores_))], fs.scores_)
plt.show()
```

```
Feature 0: 1.875144
Feature 1: 7.912676
Feature 2: 0.635834
Feature 3: 5.311644
```



We will then return from the above computation the categorical features

Cat_Features= [‘tissue’, ‘level.ribo’].

3.3 Boolean features selection

- We encode boolean features into numerical ones: False=0, True=1

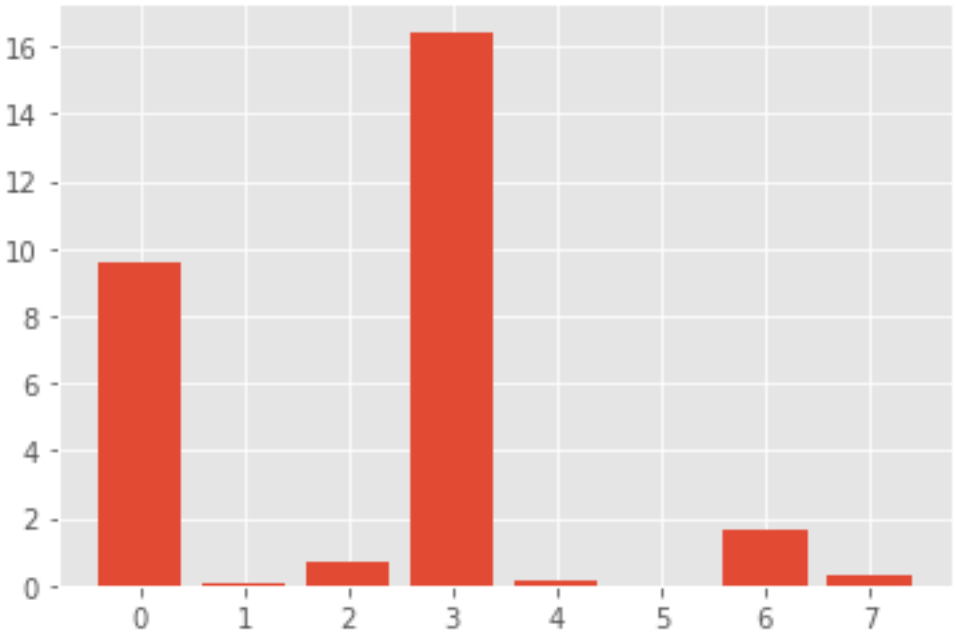
```
bool_cat= train_df.loc[:,train_df.dtypes==np.bool].astype(int)
```

- We use the ch2 method to select useful boolean features.

The boolean features of our data set are: low.yield, marker.A, marker.B, marker.C, marker.D, marker.E, marker.F, marker.G .

```
from sklearn.feature_selection import SelectKBest, chi2
import matplotlib.pyplot as plt

fs=SelectKBest(score_func=chi2, k='all')
fs.fit(bool_cat, y)

for i in range(len(fs.scores_)):
    print('Feature %d: %f' %(i, fs.scores_[i]))

# Plot the scores
plt.bar([i for i in range(len(fs.scores_))], fs.scores_)
plt.show()
```

```
Feature 0: 9.597669
Feature 1: 0.101460
Feature 2: 0.705304
Feature 3: 16.425240
Feature 4: 0.133561
Feature 5: 0.000063
Feature 6: 1.619419
Feature 7: 0.276285
```



We will then retain from the above computation the categorical features

bool_Features= ['low.yield', 'marker.C'].

3.4 Automating feature selection for a new input data

The data to consider after this process is the combination of the numerical, categorical and boolean selected features.

```
Features= ['low.yield', 'marker.C']+['tissue', 'level.ribo']+Num_Features

def transformed_data(data):
    New_data=data[Features]
    # Encode boolean features into numeric
    New_data.loc[:,New_data.dtypes==np.bool]= New_data.loc[:,New_data.dtypes==np.
 ↪bool].astype(int)
    # Encode categorical features into numeric
    New_data['tissue'], uniques_tissue=pd.factorize(New_data['tissue'])
    New_data['level.ribo'], uniques_level_ribo=pd.factorize(New_data['level.
 ↪ribo'])
    # Fill missing values with column median
    num_data= New_data.loc[:,(New_data.dtypes==np.float64) | (New_data.
 ↪dtypes==np.int64)]
    New_data.loc[:,(New_data.dtypes==np.float64) | (New_data.dtypes==np.
 ↪int64)]=num_data.fillna(num_data.median())
```

```
    return New_data



X= transformed_data(train_df)
y=train_df['label']
```

4 Model selection

In this section, we train the Ramdom Forest, SVM-classification (SVC), KNN and Gradient Boosting models. We tune the meta-parameters to obtain the best version of each model.

4.1 Random Forest model

- Tuning the model to find the best parameters

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import GridSearchCV
clf = RandomForestClassifier(max_depth=1, random_state=0)

param_grid = {
    'n_estimators': [200,300,500],
    'max_features': [.5,.7],
    'bootstrap': [False, True],
    'max_depth':[3,6]
}

model_rf = GridSearchCV(estimator=clf, param_grid=param_grid,
                        scoring=BCR_score, cv=5)

model_rf.fit(X, y)
print(model_rf.best_params_)
```

```
{'bootstrap': False, 'max_depth': 6, 'max_features': 0.7, 'n_estimators': 500}
```

- Building the random forest model

```
from sklearn.model_selection import cross_val_score

# Building the model
rf_clf = RandomForestClassifier(max_depth=6, max_features= 0.7, random_state=0,␣
 ↪bootstrap=False, n_estimators= 500)

# Get the score of the above built model
rf_score= cross_val_score(rf_clf, X, y, cv=10, scoring= BCR_score)
```

4.2 Support vector machine model

- Tuning the model to find the best parameters

```
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

param_grid = {
    'kernel': ['poly', 'rbf', 'sigmoid'],
    'gamma': ['scale', 'auto'],
    'C': [5, 1,2,3, 0.001, 0.01, .1, 10, 100]
}

model_svm = GridSearchCV(estimator=SVC(), param_grid=param_grid,
                      scoring=BCR_score, cv=5)

model_svm.fit(X, y)
print(model_svm.best_params_)
```

```
{'C': 5, 'gamma': 'scale', 'kernel': 'poly'}
```

- Building the SVM model

```
# Building the model
svm_clf = SVC(C=5, gamma= 'scale', kernel='poly')

# Get the score of the above built model
svm_score= cross_val_score(svm_clf, X, y, cv=10, scoring= BCR_score)
```

4.3 KNN model

- Tuning the model to find the best parameters

```
from sklearn.neighbors import KNeighborsClassifier

param_grid = {
    'n_neighbors': [2,3,4,5,10,20],
    'weights': ['uniform', 'distance'],
}

model_knn = GridSearchCV(estimator=KNeighborsClassifier(), param_grid=param_grid,
                      scoring=BCR_score, cv=5)
model_knn.fit(X, y)
print(model_knn.best_params_)
```

```
{'n_neighbors': 10, 'weights': 'uniform'}
```

- Building the KNN model

```
# Building the model
knn_clf = KNeighborsClassifier(n_neighbors=10, weights= 'uniform' )

# Getting the score of the above built model
knn_score = cross_val_score(knn_clf, X, y, cv=10, scoring= BCR_score)
```

4.4 Gradient Boosting model

- Tuning the model to find the best parameters

```
from sklearn.ensemble import GradientBoostingClassifier

param_grid = {
    'loss': ['deviance', 'exponential'],
    'n_estimators': [100,200,400],
    'max_features': ['auto', 'sqrt', 'log2'],
    'max_depth': [1,3,6]
}



model_GB = GridSearchCV(estimator=GradientBoostingClassifier(random_state=0),␣
 ↪param_grid=param_grid,
                        scoring=BCR_score, cv=5)
model_GB.fit(X, y)
print(model_GB.best_params_)
```

```
{'loss': 'deviance', 'max_depth': 6, 'max_features': 'auto', 'n_estimators':
200}
```

- Building the Gradient Boosting model

```
# Building the model
gb_clf = GradientBoostingClassifier(random_state=0, loss= 'deviance', max_depth=␣
 ↪6 ,max_features='auto', n_estimators= 200 )

# Getting the score of the above built model
gb_score= cross_val_score(gb_clf, X, y, cv=10, scoring= BCR_score)
```

5 Algorithms performance assessment

Algorithm performance assessment is crucial in Machine Learning and one of the mathematical tools behind this task is the Central Limit Theorem which says roughly that re-sampling the data several (many) times and computing the model score conduct on average to the true model score. In our case, we performed a 10-fold cross validation for our 4 models.

```
Score= pd.DataFrame()
Score['Random_Forest']=rf_score
Score['SVM']=svm_score
Score['KNN']=knn_score
Score['Gradient_Boosting']=gb_score
Score.loc['mean']=Score.mean()
print(Score)
```

```
      Random_Forest     SVM     KNN  Gradient_Boosting
0         -0.833333 -0.4450 -0.4450          -0.833333
1         -0.805861 -0.4450 -0.4450          -0.973404
2         -0.796099 -0.4450 -0.4450          -0.884752
3         -0.671275 -0.4450 -0.4450          -0.958763
4         -0.827778 -0.4450 -0.4450          -0.847826
5         -0.697917 -0.4400 -0.4400          -0.857895
6         -0.647368 -0.4400 -0.4400          -0.697917
7         -0.896313 -0.4400 -0.4400          -0.963158
8         -0.742704 -0.4400 -0.4400          -0.879433
9         -0.910326 -0.4400 -0.4400          -0.910326
mean      -0.782897 -0.4425 -0.4425          -0.880681
```

We deduce from this plot that the best algorithm is Gradient Boosting with an expected BCR score ~ 0.88 . On the other hand, the SVM and KNN algorithms perform poorly.

6 Prediction

Now that we have an algorithm that suit the best with the data, we can now make the prediction for new users.

```
# Loading the data
test_df=read_csv("/Users/miradain/Desktop/Machine_Learning_Q2/ML-A5-2020_test.
 ↪csv", index_col=0)

# Get the transformed data from the feature selection analysis
test_data= transformed_data(test_df)

# Train and make the prediction
gb_clf.fit(X,y)
y_pred = pd.DataFrame(gb_clf.predict(test_data))

# Save the prediction in csv file
y_pred.to_csv("/Users/miradain/Desktop/Machine_Learning_Q2/pred.csv", index =␣
 ↪False)
```

Here below is the distribution of the predicted values

```
y_pred[0].astype(str).value_counts()
```

```
-1    465
1      35
Name: 0, dtype: int64
```

The percentages of this classification are: 7% T-reg (+1) and 93% T-helper (-1).

7 Conclusion

The goal of this report was to solve a machine learning classification problem. The data set had too many features (more than 23000), therefore one of the challenges part of this research was to extract the best ones suitable to deploy our model. The data was also unbalanced, so we change the evaluation metric to tackle this issue. The best model turned out to the Gradient Boosting with an expected score of 0.88 .The SVM and KNN models perform poorly and are even bad than the canonical "majority vote" strategy.