Automatic classification and clustering of biology documents

When designing an automatic classifier, the first thing to do is insect the data to ensure the following:

- 1. You understand how the data is represented
- 2. There is enough data to train with.
- 3. There is roughly the same amount of data for each label

When inspecting the datasets (Dataset 1 - Negative and positive abstracts) and (Dataset 2 - Alzheimer, Breast cancer, Bladder cancer, Cervical Cancer and non-relevant abstracts), the data set up with the following; Document number, Document Title, Abstract. The dataset 1 contains 8156 documents and dataset 2 contains 5000 documents, all documents are evenly split among the labels.

Part I. Construction of an automatic classifier

Pre-processing is the first step in handling the data. The data is cleaned by converting all letters to lower case, removing stop words which provide no classifying formation for the classifier and splitting the documents into words. This is achieved by a simple regular expression shown in Figure 1 below

The data was then split into 70/30 train/test. The classifiers will be trained using the train data and the accuracy and performance of each classifier will be tested using the test data. For this problem, four classifiers are built in order to test which will give the best results. These can be seen in Figure 2 below.

```
classifier_NB = Pipeline([('Tfidf', TfidfVectorizer(min_df=min_df,
                                                 max df=max df.
                                                 stop words = stop words,
                                                 max_features= max_features,
                                                 norm = norm,
                                                 lowercase=False)),
                       ('LSA', TruncatedSVD(n_components = n_components)),
                       ('scaler', StandardScaler()),
                       ('NB', GaussianNB())])
classifier_SVC = Pipeline([('Tfidf', TfidfVectorizer(min_df=min_df,
                                                 max_df=max_df,
                                                 stop_words = stop_words,
                                                 max_features= max_features,
                                                 norm = norm,
                                                 lowercase=False)),
                       ('LSA', TruncatedSVD(n_components = n_components)),
                       ('scaler', StandardScaler()),
                       ('SVC', SVC(C = 1))])
classifier_KNN = Pipeline([('Tfidf', TfidfVectorizer(min_df=min_df,
                                                 max df=max df,
                                                 stop_words = stop_words,
                                                 max_features= max_features,
                                                 lowercase=False)),
                       ('LSA', TruncatedSVD(n_components = n_components)),
                       ('scaler', StandardScaler()),
                       ('KNN', KNeighborsClassifier(n_neighbors = 10))])
classifier_tree = Pipeline([('Tfidf', TfidfVectorizer(min_df=min_df,
                                                 max_df=max_df,
                                                 stop_words = stop_words,
                                                 max_features= max_features,
                                                 norm = norm.
                                                 lowercase=False)),
                       ('LSA', TruncatedSVD(n components = n components)),
                       ('scaler', StandardScaler())
                       ('tree', DecisionTreeClassifier(max_depth= 7))])
```

Figure 1 - Pipeline for building the classifier

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In order to test the effectiveness of each classifier, they will be compared to the default values of the classifiers. These are the values listed in the sklearn documentation. To try and maximize the quality of the classifiers, the following parameters were changed:

Parameter	Values							
Parameter	Default 1		2	3				
	TfidfVectorizer							
stop_words	english	None						
Max_features	200	500	2000	5000				
min_df	0.2	0.05	0.15	0.2				
max_df	0.8	0.3	0.6	0.9				
norm	l1	12	None					
LSA								
n_components	20	10	30	50				
LSA	With LSA	No LSA						

Figure 2 - Parameters for classifiers.

Note 1: The stop words were provided from nltk.corpus.

Note 2: When no LSA was used, scaler = StandardScaler(with mean=False)

The accuracy for each classifier was calculated using accuracy_score from sklearn.metrics. From the formula in figure 3, the fraction of true predictions divided by the number of samples equals the accuracy. The maximum score is 1 (perfect prediction) and the lowest is 0 (no correct predictions)

$$\mathtt{accuracy}(y, \hat{y}) = rac{1}{n_{ ext{samples}}} \sum_{i=0}^{n_{ ext{samples}}-1} 1(\hat{y}_i = y_i)$$

Figure 3 - Accuracy score formula

The Results

Below are the results for the two and five datasets. In figure 4, we can see from the default values, the best classifier is C-Support Vector Classification (SVC) with an accuracy value of 0.953, and the worst is K Nearest Neighbors (KNN) with an accuracy of 0.899. As the parameters change, there is no real change of results across the classifiers however, for the Decision Tree (tree) and Naive Bayes (NB) classifiers, they see the biggest change in accuracy when they are not dimensionality reduction using truncated SVD (LSA). This would indicate that when using these classifiers, you would be required to reduce dimensions to achieve the optimal results. The best scores for each classifier are highlighted in green with the overall best score being SVC min_df = 0.05.

The results for the 5-label dataset are less accurate but again the best classifier here is SVC with 0.8373 (min_df = 0.05). Looking specifically at the No-LSA result for KNN, at 0.4693, it is 36% lower than the best result indicating that now with 5 labels, dimension reduction is far more important than it was before in the 2-label data.

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The classification report shows the fraction of true positive results for both datasets. We can see that there is a higher score (0.95) for the 2-label dataset compared to the 5-label dataset (0.82). The differences in the scores could be due to the fact that the 2-label dataset has more documents compared to the 5-label dataset. Potentially including more documents in the 5-label classifier could improve its ability to classify correctly.

2 label dataset							
Parameter	Value	Tree	NB	SVC	KNN		
TfidfVectorizer							
Default	Default	0.9428	0.9252	0.9526	0.8991		
stop_words	none	0.9354	0.9273	0.9497	0.9027		
	200	0.9367	0.9273	0.9555	0.9027		
Max features	500	0.9403	0.9260	0.9538	0.9003		
iviax_leatures	2000	0.9354	0.9252	0.9510	0.9044		
	5000	0.9407	0.9256	0.9555	0.9036		
	0.05	0.9338	0.9256	0.9563	0.9064		
min_df	0.15	0.9362	0.9273	0.9530	0.9019		
	0.2	0.9391	0.9244	0.9555	0.9011		
	0.3	0.9367	0.9289	0.9522	0.8966		
max_df	0.6	0.9412	0.9260	0.9546	0.9019		
	0.9	0.9383	0.9236	0.9542	0.9040		
norm	L2	0.9399	0.9252	0.9522	0.8987		
norm	none	0.9403	0.9268	0.9534	0.9031		
LSA							
n_components	10	0.9371	0.9264	0.9534	0.8999		
	30	0.9350	0.9224	0.9522	0.9011		
	50	0.9395	0.9256	0.9510	0.9064		
no_LSA	removed	0.9125	0.9040	0.9363	0.9093		

5 label dataset							
Parameter	Value	Tree	NB	SVC	KNN		
TfidfVectorizer							
Default	Default	0.6687	0.7307	0.8340	0.7333		
stop_words	none	0.6633	0.7353	0.8333	0.7320		
	500	0.6760	0.7347	0.8340	0.7293		
max_features	2000	0.6660	0.7307	0.8333	0.7320		
	5000	0.6787	0.7327	0.8353	0.7353		
min_df	0.05	0.6500	0.7393	0.8373	0.7340		
	0.15	0.6640	0.7320	0.8347	0.7333		
	0.2	0.6833	0.7307	0.8327	0.7293		
	0.3	0.6653	0.7400	0.8327	0.7360		
max_df	0.6	0.6567	0.7300	0.8360	0.7273		
	0.9	0.6600	0.7313	0.8347	0.7300		
n o rm	L2	0.6640	0.7333	0.8353	0.7300		
norm	none	0.6940	0.7320	0.8333	0.7353		
LSA							
n_components	10	0.6600	0.7367	0.8367	0.7333		
	30	0.6653	0.7300	0.8340	0.7353		
	50	0.6927	0.7287	0.8293	0.7307		
no_LSA	removed	0.8900	0.7287	0.8033	0.4693		

Figure 4 - Scores for 2 label dataset (left)-and 5 label dataset (right). Best scores are highlighted in green

	precision	recall	f1-score	support		precision	recall	f1-score	support
					Cbladder	0.83	0.79	0.81	282
neg	0.96	0.94	0.95	1234	Cbreast	0.84	0.75	0.79	306
_	0.94	0.96	0.95	1213	Ccervix	0.90	0.79	0.84	315
pos	0.54	0.96	0.95	.95 1213	alz	0.94	0.84	0.88	293
avg / total	0.95	0.95	0.95	2447	neg	0.62	0.85	0.72	304
					avg / total	0.82	0.80	0.81	1500

Figure 5 - Classification score for 2 label dataset (left)-and 5 label dataset (right). Classifier: SVC, Parameters: Best from figure 4

Tips for construction an automatic classifier:

From both datasets, the min_df gave the best results for SVC. The stop_words and max_features give similar results regardless of the change. To further tune the classifiers, I would continue to look into getting the optimal min_df.

Choosing the parameters for the classifier depends a lot on the type of data you are working with. As both datasets were different, simply choosing parameters that worked for one dataset may not work well for another. Therefore, I would recommend analyzing the classification problem first before

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jumping into building the classifier. Although SVC gave the best scores in both cases, there could be a better classifier suited for the 5-label dataset.

Part II. Construction of a clustering of biology documents

This is a slightly different problem from above. We already know the classes for the datasets but this time we want to see how well the clustering program can group the documents together without knowing the class. For this problem, we will not use the class in training the program but we will call it later to determine the accuracy of the clustering. The data will also not be split into training and test. As we are performing unsupervised clustering, all the data will be used in developing the clustering program.

Below is the code used for building the clustering program. The number of components changes depending if we are working with the 2 or 5 label datasets. In order to change the vocabulary size, the number of features was altered.

```
def preprocessing(line):
   line = line.lower()
   line = re.sub(r"[{}]".format(string.punctuation), " ", line)
   return line
tfidf_vectorizer = TfidfVectorizer(preprocessor=preprocessing,
                                  max_features=max_features, #1
                                  norm = norm, #2
                                  lowercase=False)
tfidf = tfidf vectorizer.fit transform(X)
LSA = TruncatedSVD(n_components = n_components, #3
                  random_state = 0)
LSAX = LSA.fit_transform(tfidf) #4
scaler = StandardScaler()
scaX = scaler.fit_transform(LSAX)
normalizer = Normalizer() #5
NX = normalizer.fit_transform(scaX)
```

Figure 6 – Code for building the clustering program

Parameter	Values						
Parameter	Default 1		2	3			
TfidfVectorizer							
stop_words	english	None					
Max_features	500	2000	5000	10000			
norm	l1	12	None				
LSA							
n_components	20	10	30	50			
LSA	With LSA	No LSA					

Figure 7 - Parameters for clustering.

Note 3: The stop words were provided from nltk.corpus.

Note 4: When no LSA was used, scaler = StandardScaler(with_mean=False)

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What is K-means?

Form the sklearn documentation on K-means, this algorithm aims to find the centroid to a predetermined number of clusters. With this centroid, it will cluster all the points are nearest to it. The centroid is chosen in order to minimize the within-cluster sum of squares criterion. This is given by the formula below:

$$\sum_{i=0}^n \min_{\mu_j \in C} (||x_i-\mu_j||^2)$$

Figure 8 - Formula used in K-means

K-means does have limitations in its use.

- 1. Data must have no missing values. If there is missing data in the dataset, it should either be removed entirely or estimated based on the data from the dataset.
- 2. K-means responds poorly to elongated clusters or clusters with irregular shapes
- 3. Depending where the initialization of the first centroid is, K-means can converge on different locations, thus giving different clusters. A method to address this is the use of the parameter init='k-means++'. This tries to ensure that the centroids are always initialized at a distance from each other rather than randomly initializing them which could place them close together.

What is Ward?

Ward is a method of hierarchical clustering. This type of clustering aims to create a tree with the cluster as the root and the leaves as the unique samples. Ward is a type of merge strategy that aims to minimize the sum of the squared difference within all clusters. Similar to K-means, this is a variance minimizing approach. This type of hierarchical clustering also outputs a tree where the distribution of the documents can be seen.

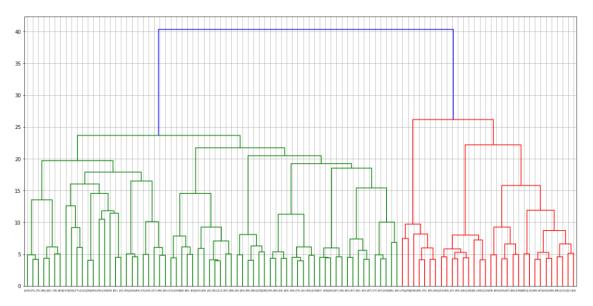


Figure 9 - Example of dendrogram from hierarchical clustering

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The results:

Figure 8 below represents the results for the clustering using two different algorithms. K-means and Ward. In a perfect scenario, the clustering would be Cluster0 = 50 pos and Cluster1 = 50 neg (or vice versa).

For K-means, the results are fairly consistent across all the parameter changes, with No LSA giving the best result. When looking at the Ward results, these are less successful. Ward appears to group the majority of the documents into one cluster every time, with the best results for no normalization. Without the prior labels to train the clustering program, it has a harder time to achieve good results compared to the classifier above.

Clustering							
2 label dataset							
		K me	eans	Ward			
Parameter	Value	Cluster 0	Cluster 1	Cluster 0	Cluster 1		
TfidfVectorizer							
Default		7.4301	42.5699	13.7200	36.2800		
Delauit	Default	49.8406	0.1594	49.5954	0.4046		
		7.4792	42.5208	17.3982	32.6018		
	500	49.8283	0.1717	49.8038	0.1962		
May footures		42.4105	7.5895	22.6336	27.3664		
Max_features	2000	0.1226	49.8774	0.0245	49.9755		
		7.3811	42.6189	13.0947	36.9053		
	5000	49.8651	0.1349	49.8038	0.1962		
Normalization		8.3619	41.6381	41.0741	8.9259		
NOTITIALIZACION	None	49.5586	0.4414	2.0721	47.9279		
		7.4792	42.5208	15.9392	34.0608		
и о и и и	L2	49.8529	0.1471	49.6935	0.3065		
norm		7.4792	42.5208	15.9392	34.0608		
	None	49.8529	0.1471	49.6935	0.3065		
		LSA					
		7.1849	42.8151	12.9475	37.0525		
n_components	10	49.8406	0.1594	49.1663	0.8337		
		7.8225	42.1775	15.5346	34.4654		
	30	49.8529	0.1471	0.0736	49.9264		
		7.9819	42.0181	19.7401	30.2599		
	50	49.8529	0.1471	49.3747	0.6253		
no 15A		7.9819	42.0181	NA	NA		
no_LSA	None	49.8529	0.1471	NA	NA		

Figure 10 - Scores for 2 label dataset (left)-and 5 label dataset (right). Negative documents are highlighted in yellow, positive documents are in white. Cells with NA could not attain a result

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The results for the dataset with 5 labels were worse than those compared to 2 labels. Below is an example of the output. In the majority of clusters, there is no clear dominance of any particular document type. This shows the difficulty the clustering algorithm had in separating the documents by type.

```
- Cluster 0
                                - Cluster 0
                                  15.12% of total patterns
  37.78% of total patterns
                                Cbladder : 2.26
Cbladder : 10.22
                                Cbreast : 4.9
Cbreast : 8.58
                                Ccervix : 3.34
Ccervix : 9.139999999999999
                                alz : 1.98000000000000000
alz : 6.88
                                neg : 2.64
neg : 2.96
- Cluster 1
                                - Cluster 1
  16.26% of total patterns
                                 13.76% of total patterns
                                Cbladder: 0.04
Cbladder : 5.08
                                Cbreast : 0.06
Cbreast : 3.479999999999999
                                Ccervix : 0.02
Ccervix : 4.5
                                alz : 12.82
alz: 0.64
                                neg : 0.82000000000000001
neg : 2.56
- Cluster 2
                                - Cluster 2
  13.4% of total patterns
                                  14.3% of total patterns
Cbladder : 0.4
                                Cbladder : 2.719999999999998
Cbreast: 0.64
                                Cbreast : 1.64000000000000001
                                Ccervix : 2.12
Ccervix: 0.18
                                alz : 1.70000000000000000
alz : 9.46
                                neg : 6.12
neg : 2.719999999999998
- Cluster 3
                                - Cluster 3
  13.22% of total patterns
                                  8.04% of total patterns
Cbladder : 2.64
                                Cbladder : 3.62
Cbreast : 4.82
                                Cbreast: 0.48
Ccervix : 3.82
                                Ccervix : 1.94
                                alz : 0.18
alz : 0.4599999999999999
                                neg : 1.82
neg : 1.48
- Cluster 4
                                - Cluster 4
  19.34% of total patterns
                                  48.78% of total patterns
Cbladder : 1.66
                                Cbladder : 11.3600000000000001
Cbreast: 2.48
                                Cbreast : 12.9200000000000000
Ccervix : 2.36
                                Ccervix : 12.58
alz : 2.56
                                alz : 3.32
neg : 10.2800000000000001
                                neg : 8.6
```

Figure 4 - Results for 5-label dataset. K-means(left) Hierarchical clustering-ward (right)