Introduction to Machine Learning

Work 2

Dimensionality reduction with PCA and Visualization using Principal Component Analysis and UMAP

Contents

1 Description of the work

The aim of the exercise is to analyze with Principal Component Analysis and UMAP algorithms in several data sets from the UCI repository. To this end, first of all you will implement the principal component analysis algorithm using **Python 3.7**.

1.1 Methodology of the analysis

You will analyze the behavior of the principal component analysis (PCA) algorithm and the Uniform Manifold Approximation and Projection for Dimension Reduction (UMAP) algorithm in well-known data sets from the UCI repository. These data sets are defined in **.arff** format. Use the parser implemented in previous work to read the .arff file in Python and save the information in a matrix.

The work is divided into several parts:

1. Implement **your own** Principal Component Analysis algorithm in Python. You **cannot** use the PCA code that exists in *sklearn* library or any other one. You will implement it in several steps:
   - Step 1. Read the .arff file and take the whole data set consisting of d-dimensional samples ignoring the class labels. Save the information in a matrix.
   - Step 2. Plot the original data set (choose two or three of its features to visualize it).
   - Step 3. Compute the d-dimensional mean vector (i.e., the means of every dimension of the whole data set).
   - Step 4. Compute the covariance matrix of the whole data set. Show this information.
   - Step 5. Calculate eigenvectors (e_1, e_2, …, e_d) and their corresponding eigenvalues of the covariance matrix. Use *numpy* library. **Write them in console**.
   - Step 6. Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors with the largest eigenvalues to form a new d x k dimensional matrix (where every column represents an eigenvector). Write the sorted eigenvectors and eigenvalues in console.
   - Step 7. Derive the new data set. Use this d x k eigenvector matrix to transform the samples onto the new subspace.
   - Step 8. Plot the new subspace (choose the largest eigenvectors to plot the matrix).
   - Step 9. Reconstruct the data set back to the original one. Additionally, plot the data set.

2. Analyze your PCA algorithm in three data sets (see Section 2). You will continue with the datasets chosen in the previous work. If you want to modify your previous selection, send an email explaining why you need to do this change to maria.salamo@ub.edu.

3. Compare and analyze your results to the ones obtained using *sklearn.decomposition.PCA* and *sklearn.decomposition.IncrementalPCA* library.

4. Use PCA to reduce the dimensionality of your data sets and cluster it with the K-Prototypes or the K-Means algorithm implemented in Work 1. Compare your new results with the ones obtained previously.

5. Visualize in low-dimensional space. You need to visualize your original data sets, the result of the K-Prototypes or K-Means algorithm without the dimensionality reduction, and the result of the K-Prototypes or K-Means algorithm with the dimensionality reduction. To visualize in a low-dimensional space (2D or 3D) you will use: PCA and UMAP (use the *umap-learn* library to do it, no other library is allowed). You will find useful information of how to deal with this algorithm at: https://umap-learn.readthedocs.io/en/latest/index.html.

1.2 Work to deliver

In this work, you will implement your own code for PCA and analyze both PCA and UMAP algorithms. You may select 3 data sets (the ones chosen in Work 1) for your analysis. At the end, you will find again the list of the data sets available (see Section 2).

The idea is that you implement **your own code in Python 3.7 and PyCharm IDE** and you will use it to produce the results of the analysis.

Once you have obtained the results, you will show them in several ways:

1. Plot the figures of the data sets (original data set and transformed data set).
2. Show the information of the original matrix, the covariance matrix, eigenvectors, eigenvalues, and the transformed data set onto the new subspace.
3. Plot the results of the K-Prototypes/K-Means with original variables, K-Prototypes/K-Means with dimensionality reduction, using PCA and UMAP.

From the outputs and plots, you will reason and extract conclusions about the results obtained. For example, some questions that may help you to comment your results:

- Is PCA giving you more advice for knowing the underlying information in the data set?
- Can you explain the setup that you have used for PCA algorithm?
- Can you reduce the dimensionality of the data set? In case of an affirmative answer, detail how do you do and how many features have been reduced from the original data set.
- Do you obtain the same results from your code to the code in `sklearn`? Explain the similarities and the differences among the two implementations.
- Can you explain if you obtain similar clusters with the data set reduced to those obtained in the original data? In addition, have you observed a reduction in time?
- Which are the similarities and differences in the visualizations obtained using PCA and UMAP algorithms?

You should deliver a report as well as the code in Python 3.7 and Pycharm project in Racó in a zip file by November, 22th 2021. The name of the zip file must contain name and surname of every member of the group.

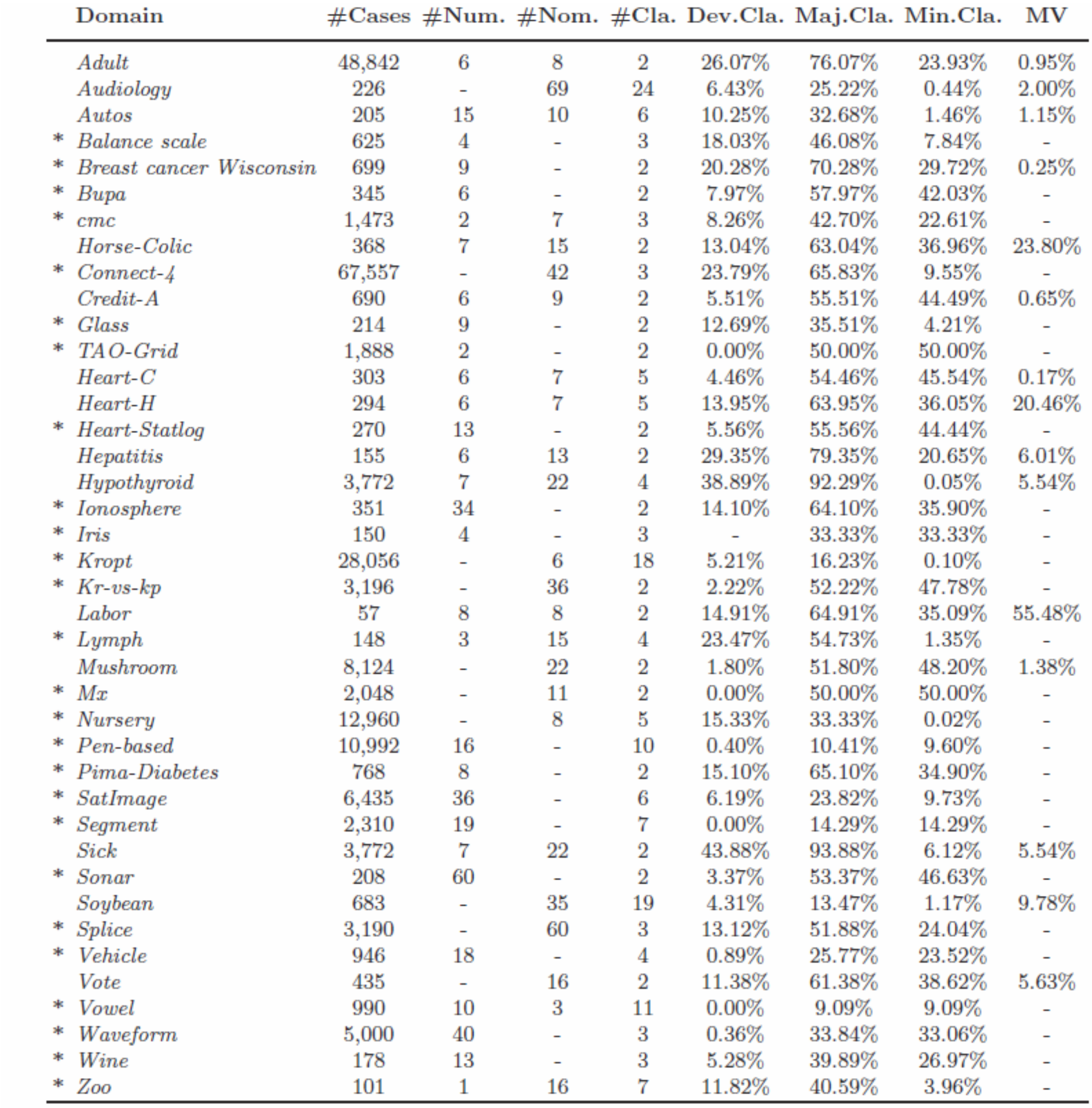
The report will contain:

- Details about the implementation of your algorithms, including the decisions made during the implementation and the setup of the different parameters.
- The evaluation of the algorithm, including outputs in console and graphs that show your results with comments about them.
- Reason each one of the questions defined above in your evaluation and add any comment or observation that you consider important from your results.
- **Additionally, you should explain how to execute your code.**

- In this work, the maximum length of the report is **10 pages long, one column report**. Please, summarize appropriately your results.

2 Data sets

Below, you will find a table that shows in detail the data sets that you can use in this work. All these data sets are obtained from the UCI machine learning repository. First column describes the name of the domain or data set. Next columns show #Cases = Number of cases or instances in the data set, #Num. = Number of numeric attributes, #Nom = Number of nominal attributes, #Cla. = Number of classes, Dev.Cla. = Deviation of class distribution, Maj.Cla. = Percentage of instances belonging to the majority class, Min.Cla. = Percentage of instances belonging to the minority class, MV = Percentage of values with missing values (it means the percentage of unknown values in the data set). When the columns contain a '-', it means a 0. For example, the Glass data set contains 0 nominal attributes and it is complete as it does not contain missing values.



	Domain	#Cases	#Num.	#Nom.	#Cla.	Dev.Cla.	Maj.Cla.	Min.Cla.	MV
	Adult	48,842	6	8	2	26.07%	76.07%	23.93%	0.95%
	Audiology	226	-	69	24	6.43%	25.22%	0.44%	2.00%
	Autos	205	15	10	6	10.25%	32.68%	1.46%	1.15%
*	*Balance scale*	625	4	-	3	18.03%	46.08%	7.84%	-
*	*Breast cancer Wisconsin*	699	9	-	2	20.28%	70.28%	29.72%	0.25%
*	*Bupa*	345	6	-	2	7.97%	57.97%	42.03%	-
*	*cmc*	1,473	2	7	3	8.26%	42.70%	22.61%	-
	Horse-Colic	368	7	15	2	13.04%	63.04%	36.96%	23.80%
*	*Connect-4*	67,557	-	42	3	23.79%	65.83%	9.55%	-
	Credit-A	690	6	9	2	5.51%	55.51%	44.49%	0.65%
*	*Glass*	214	9	-	2	12.69%	35.51%	4.21%	-
*	*TAO-Grid*	1,888	2	-	2	0.00%	50.00%	50.00%	-
	Heart-C	303	6	7	5	4.46%	54.46%	45.54%	0.17%
	Heart-H	294	6	7	5	13.95%	63.95%	36.05%	20.46%
*	*Heart-Statlog*	270	13	-	2	5.56%	55.56%	44.44%	-
	Hepatitis	155	6	13	2	29.35%	79.35%	20.65%	6.01%
	Hypothyroid	3,772	7	22	4	38.89%	92.29%	0.05%	5.54%
*	*Ionosphere*	351	34	-	2	14.10%	64.10%	35.90%	-
*	*Iris*	150	4	-	3	-	33.33%	33.33%	-
*	*Kropt*	28,056	-	6	18	5.21%	16.23%	0.10%	-
*	*Kr-vs-kp*	3,196	-	36	2	2.22%	52.22%	47.78%	-
	Labor	57	8	8	2	14.91%	64.91%	35.09%	55.48%
*	*Lymph*	148	3	15	4	23.47%	54.73%	1.35%	-
	Mushroom	8,124	-	22	2	1.80%	51.80%	48.20%	1.38%
*	*Mx*	2,048	-	11	2	0.00%	50.00%	50.00%	-
*	*Nursery*	12,960	-	8	5	15.33%	33.33%	0.02%	-
*	*Pen-based*	10,992	16	-	10	0.40%	10.41%	9.60%	-
*	*Pima-Diabetes*	768	8	-	2	15.10%	65.10%	34.90%	-
*	*SatImage*	6,435	36	-	6	6.19%	23.82%	9.73%	-
*	*Segment*	2,310	19	-	7	0.00%	14.29%	14.29%	-
	Sick	3,772	7	22	2	43.88%	93.88%	6.12%	5.54%
*	*Sonar*	208	60	-	2	3.37%	53.37%	46.63%	-
	Soybean	683	-	35	19	4.31%	13.47%	1.17%	9.78%
*	*Splice*	3,190	-	60	3	13.12%	51.88%	24.04%	-
*	*Vehicle*	946	18	-	4	0.89%	25.77%	23.52%	-
	Vote	435	-	16	2	11.38%	61.38%	38.62%	5.63%
*	*Vowel*	990	10	3	11	0.00%	9.09%	9.09%	-
*	*Waveform*	5,000	40	-	3	0.36%	33.84%	33.06%	-
*	*Wine*	178	13	-	3	5.28%	39.89%	26.97%	-
*	*Zoo*	101	1	16	7	11.82%	40.59%	3.96%	-