

Question 1 : (30 total points) Image data analysis with PCA



















































In this question we employ PCA to analyse image data

1.1 (3 points) Once you have applied the normalisation from Step 1 to Step 4 above, report the values of the first 4 elements for the first training sample in `Xtrn_nm`, i.e. `Xtrn_nm[0,:]` and the last training sample, i.e. `Xtrn_nm[-1,:]`.

$$X_{first} \approx (-3.137, -22.680, -117.974, -407.059, \dots)^T \times 10^{-6}$$
$$X_{last} \approx (-3.137, -22.680, -117.974, -407.059, \dots)^T \times 10^{-6}$$

1.2 (4 points) Using **Xtrn** and Euclidean distance measure, for each class, find the two closest samples and two furthest samples of that class to the mean vector of the class.

**Mean, closest and furthest samples for each class
(indices on top of images)**

	Mean	Closest #59933	2nd Cl. #25846	2nd Fur. #20348	Furthest #51163
Class #0		 #13767	 #18720	 #43178	 #56855
Class #1		 #3518	 #53758	 #53579	 #18913
Class #2		 #28687	 #36680	 #53509	 #14842
Class #3		 #30335	 #43937	 #17267	 #5346
Class #4		 #16895	 #44193	 #20982	 #18906
Class #5		 #344	 #40687	 #31587	 #55023
Class #6		 #51327	 #44957	 #13624	 #51601
Class #7		 #28998	 #28590	 #56147	 #29088
Class #8		 #32622	 #9055	 #29147	 #33141
Class #9		 #32622	 #9055	 #29147	 #33141

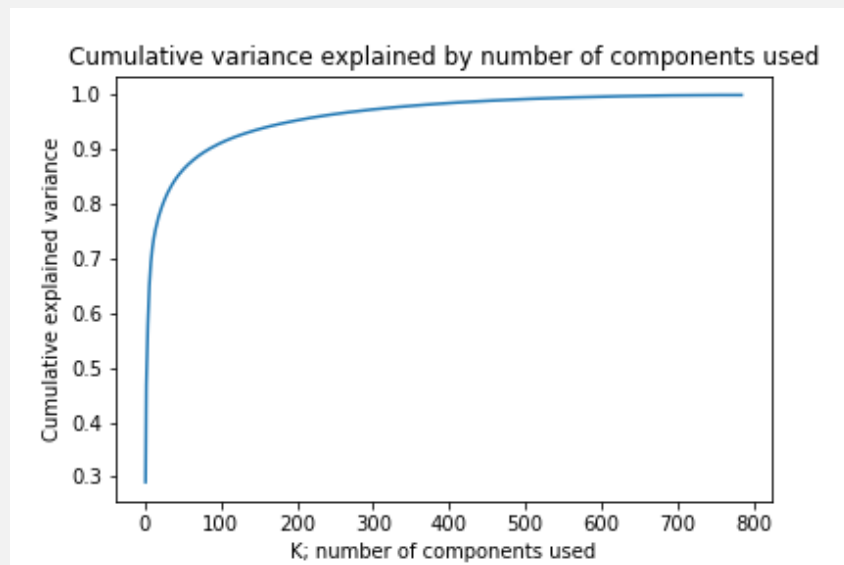
The closest samples from each class look very similar to the mean and have light colours. The furthest samples from each class are unusual examples of that class and are dark. This makes sense, as similar images will have usually smaller distances and gray deviations from mean increase the distance less than black ones do.

1.3 (3 points) Apply Principal Component Analysis (PCA) to the data of `Xtrn_nm` using `sklearn.decomposition.PCA`, and report the variances of projected data for the first five principal components in a table. Note that you should use `Xtrn_nm` instead of `Xtrn`.

PCA variances of projected data for the first 5 components:

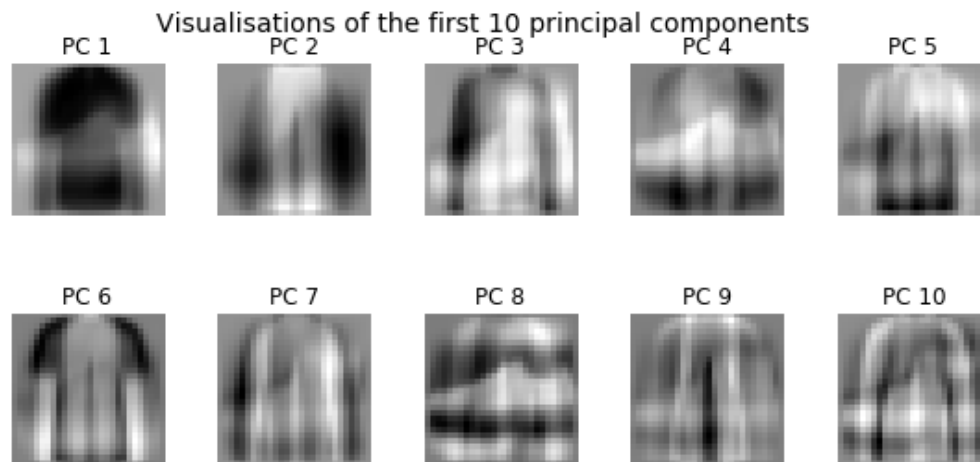
K	1	2	3	4	5
Var	19.81	12.11	4.11	3.38	2.62

1.4 (3 points) Plot a graph of the cumulative explained variance ratio as a function of the number of principal components, K , where $1 \leq K \leq 784$. Discuss the result briefly.



- We can see that the cumulative explained variance grows quickly in the $1 \leq K \leq 50$ interval. Following that, the function increases much more slowly.
- Therefore, as $K = 50$ PCA components explain $> 86\%$ of the variance, it looks like a good compromise between accuracy and complexity.
- It is often useful to plot decision regions on the plane spanned by the first 2 PCA components. They explain only $\sim 53\%$ of the total variance here, so one would need to be cautious when using them.

1.5 (4 points) Display the images of the first 10 principal components in a 2-by-5 grid, putting the image of 1st principal component on the top left corner, followed by the one of 2nd component to the right. Discuss your findings briefly.



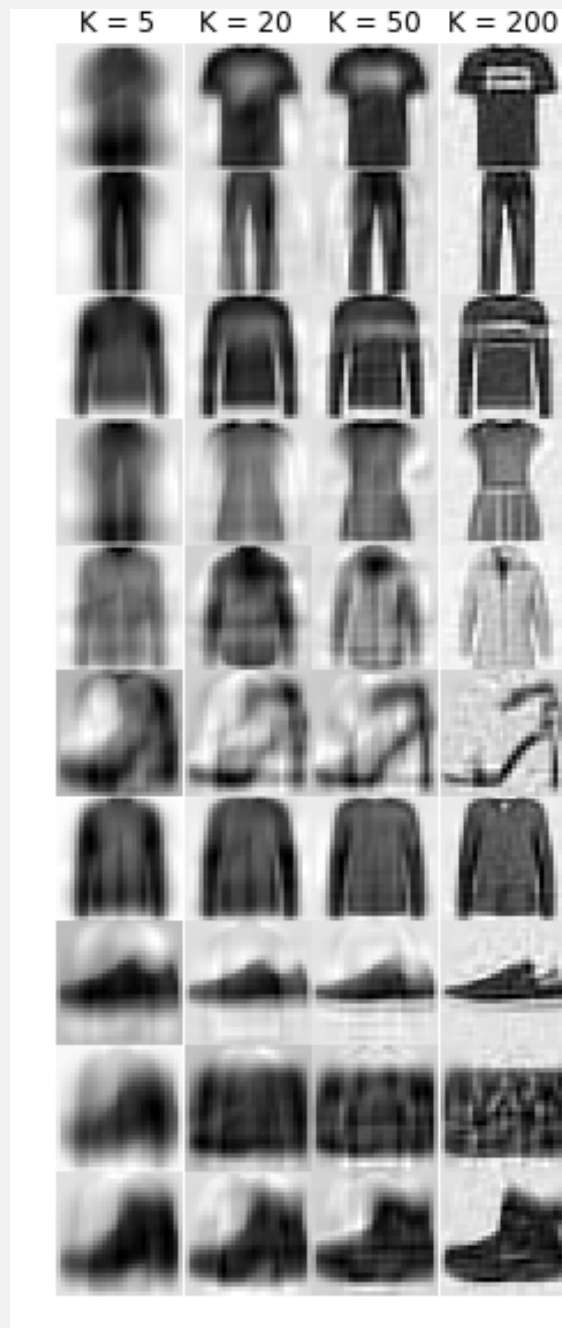
- We can see that the first component measures how much a picture resembles a shirt, as it has a shape of a t-shirt with gray areas in the shapes of sleeves. This makes sense as there are 4 classes with similar shapes (0: T-Shirt/Top, 2: Pullover, 4: Coat, 6: Shirt). These classes share a shape, so lots of variance can be explained by identifying it. Therefore, it is expected for the most important principal component to identify it (even though PCA is unsupervised).
- Out of the other principal components, we can similarly see that the 4-th and the 8-th one identify shoes (and also 5 and 10, but to a smaller degree). This makes sense, as there are 3 classes of shoes and they share a unique shape.

1.6 (5 points) Using `Xtrn_nm`, for each class and for each number of principal components $K = 5, 20, 50, 200$, apply dimensionality reduction with PCA to the first sample in the class, reconstruct the sample from the dimensionality-reduced sample, and report the Root Mean Square Error (RMSE) between the original sample in `Xtrn_nm` and reconstructed one.

RMSE between original and reconstructed samples
for $K = 5, 20, 50, 200$:

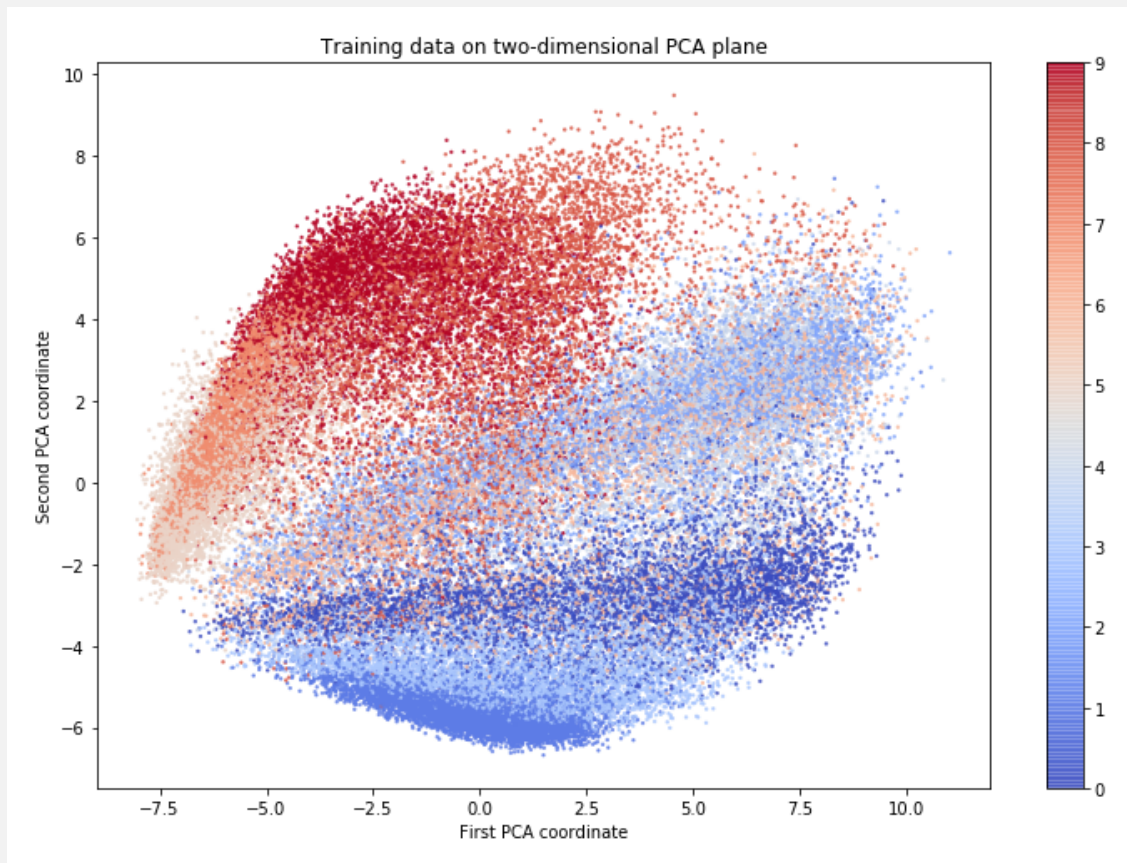
	K=5	K=20	K=50	K=200
Class #0	0.26	0.15	0.13	0.06
Class #1	0.20	0.14	0.10	0.04
Class #2	0.20	0.15	0.12	0.08
Class #3	0.15	0.11	0.08	0.06
Class #4	0.12	0.10	0.09	0.05
Class #5	0.18	0.16	0.14	0.09
Class #6	0.13	0.10	0.07	0.05
Class #7	0.17	0.13	0.11	0.06
Class #8	0.22	0.15	0.12	0.09
Class #9	0.18	0.15	0.12	0.07

1.7 (4 points) Display the image for each of the reconstructed samples in a 10-by-4 grid, where each row corresponds to a class and each row column corresponds to a value of $K = 5, 20, 50, 200$.



We should expect more components to yield better reconstructions and that is visibly the case. The more components we use, the more variance they explain. Therefore, the images should also look more and more realistic (less blurred) and they do.

1.8 (4 points) Plot all the training samples (`Xtrn_nm`) on the two-dimensional PCA plane you obtained in Question 1.3, where each sample is represented as a small point with a colour specific to the class of the sample. Use the 'coolwarm' colormap for plotting.



- The classes are not fully separated as we can, for example, see that red and blue samples mix in the middle.
- We can also observe that the bottom is dominated by blue samples and the top by red/orange ones.
- This suggests that the first PCA component has little discriminatory power (but explains more of the variance), while the second PCA component actually distinguishes between classes (given the first component).

Question 2 : (25 total points) Logistic regression and SVM

In this question we will explore classification of image data with logistic regression and support vector machines (SVM) and visualisation of decision regions.

2.1 (3 points) Carry out a classification experiment with **multinomial logistic regression**, and report the classification accuracy and confusion matrix (in numbers rather than in graphical representation such as heatmap) for the test set.

Accuracy: 84.01%

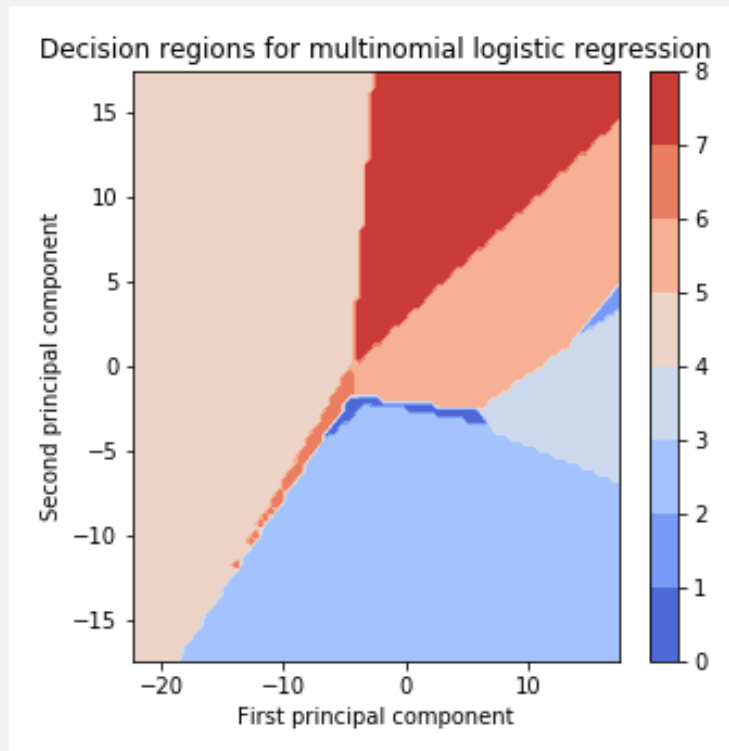
Confusion Matrix (C_{ij} = samples known to be in class i and predicted to be in j)										
	0	1	2	3	4	5	6	7	8	9
0	819	3	15	50	7	4	89	1	12	0
1	5	953	4	27	5	0	3	1	2	0
2	27	4	731	11	133	0	82	2	9	1
3	31	15	14	866	33	0	37	0	4	0
4	0	3	115	38	760	2	72	0	10	0
5	2	0	0	1	0	911	0	56	10	20
6	147	3	128	46	108	0	539	0	28	1
7	0	0	0	0	0	32	0	936	1	31
8	7	1	6	11	3	7	15	5	945	0
9	0	0	0	1	0	15	1	42	0	941

2.2 (3 points) Carry out a classification experiment with **SVM classifiers**, and report the mean accuracy and confusion matrix (in numbers) for the test set.

Accuracy: 84.61%

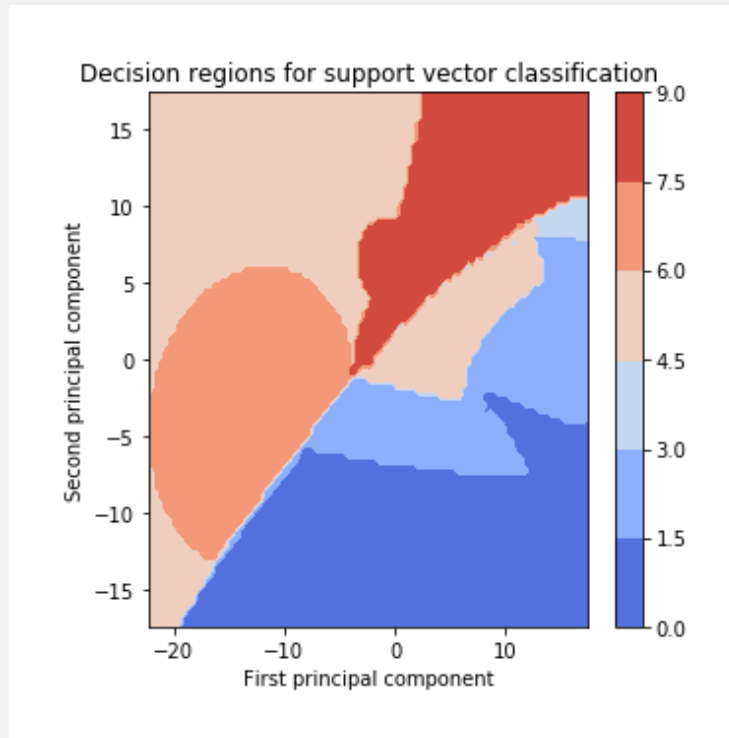
Confusion Matrix (C_{ij} = samples known to be in class i and predicted to be in j)										
	0	1	2	3	4	5	6	7	8	9
0	845	2	8	51	4	4	72	0	14	0
1	4	951	7	31	5	0	1	0	1	0
2	15	2	748	11	137	0	79	0	8	0
3	32	6	12	881	26	0	40	0	3	0
4	1	0	98	36	775	0	86	0	4	0
5	0	0	0	1	0	914	0	57	2	26
6	185	1	122	39	95	0	533	0	25	0
7	0	0	0	0	0	34	0	925	0	41
8	3	1	8	5	2	4	13	4	959	1
9	0	0	0	0	0	22	0	47	1	930

2.3 (6 points) We now want to visualise the decision regions for the logistic regression classifier we trained in Question 2.1.



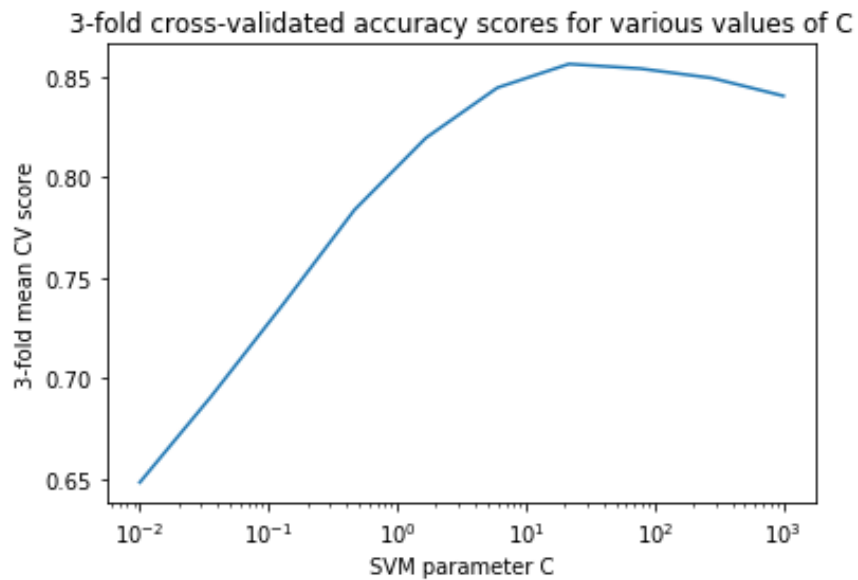
- Each class has a linear boundary here. This makes sense, as logistic regression is a linear classifier and PCA coordinates are linear combinations of original coordinates. Irregularities are probably caused by the numerical approximation.
- As expected (first two components explain most of the variance), the main differences are visibly captured.

2.4 (4 points) Using the same method as the one above, plot the decision regions for the SVM classifier you trained in Question 2.2. Comparing the result with that you obtained in Question 2.3, discuss your findings briefly.



- Unlike for logistic regression, decision boundaries here are non-linear. This makes sense as SVMs are not linear classifiers (not for RBF kernels).
- There are significant differences in decision regions between the SVM model and logistic regression.
- As expected (first two components explain most of the variance), the main differences are visibly captured here as well.

2.5 (6 points) We used default parameters for the SVM in Question 2.2. We now want to tune the parameters by using cross-validation. To reduce the time for experiments, you pick up the first 1000 training samples from each class to create `Xsmall`, so that `Xsmall` contains 10,000 samples in total. Accordingly, you create labels, `Ysmall`.



The highest mean 3-fold CV accuracy score was $\sim 85.65\%$.
It was realised by $C = 10^{4/3} \approx 21.54$.

2.6 (3 points) Train the SVM classifier on the whole training set by using the optimal value of C you found in Question [2.5](#).

Classification accuracy for $C = 10^{4/3}$ is approximately:

- 90.84% for the training data
- 87.65% for the test data

Question 3 : (20 total points) Clustering and Gaussian Mixture Models

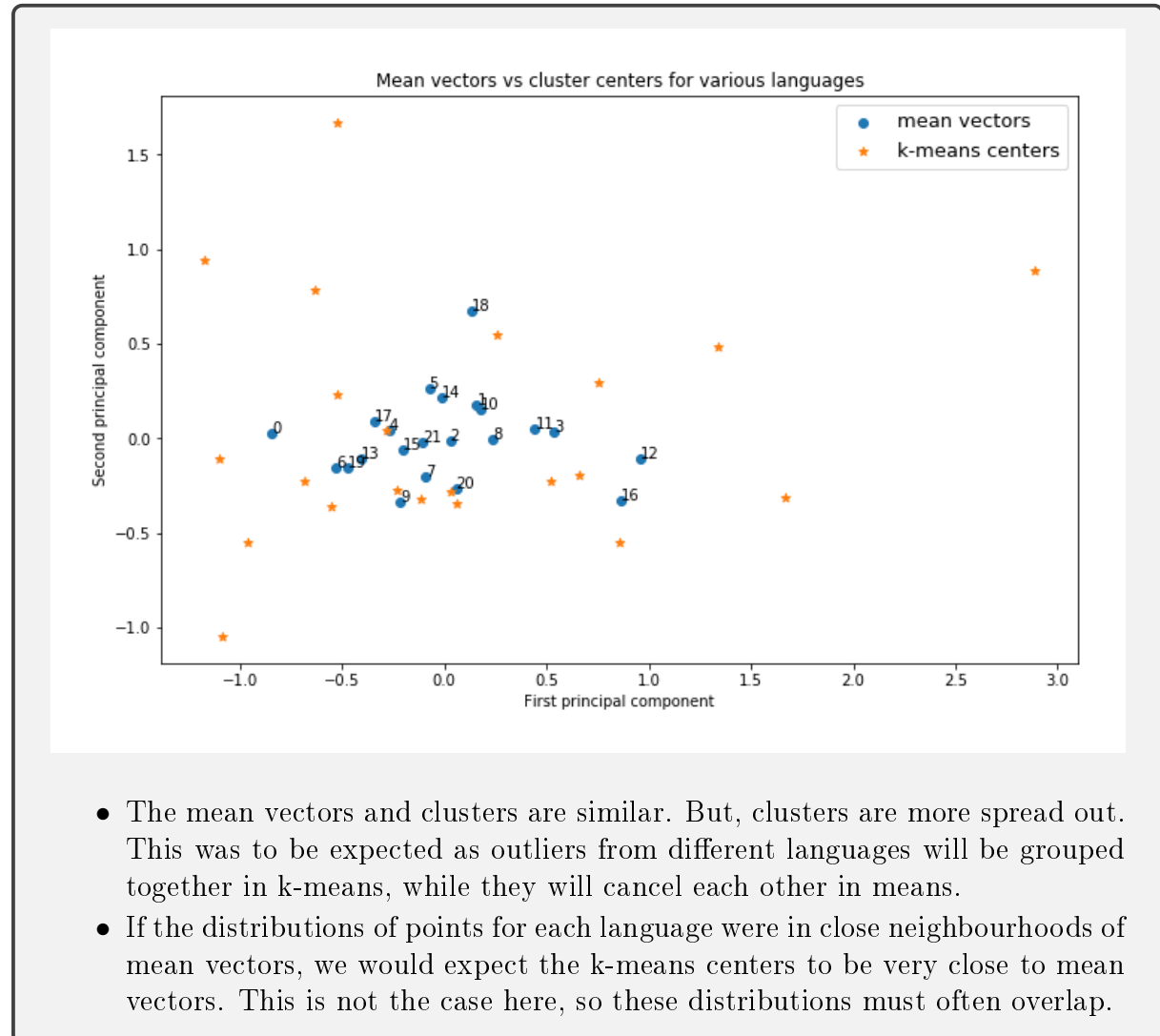
In this question we will explore K-means clustering, hierarchical clustering, and GMMs.

3.1 (3 points) Apply k-means clustering on `Xtrn` for $k = 22$, where we use `sklearn.cluster.KMeans` with the parameters `n_clusters=22` and `random_state=1`. Report the sum of squared distances of samples to their closest cluster centre, and the number of samples for each cluster.

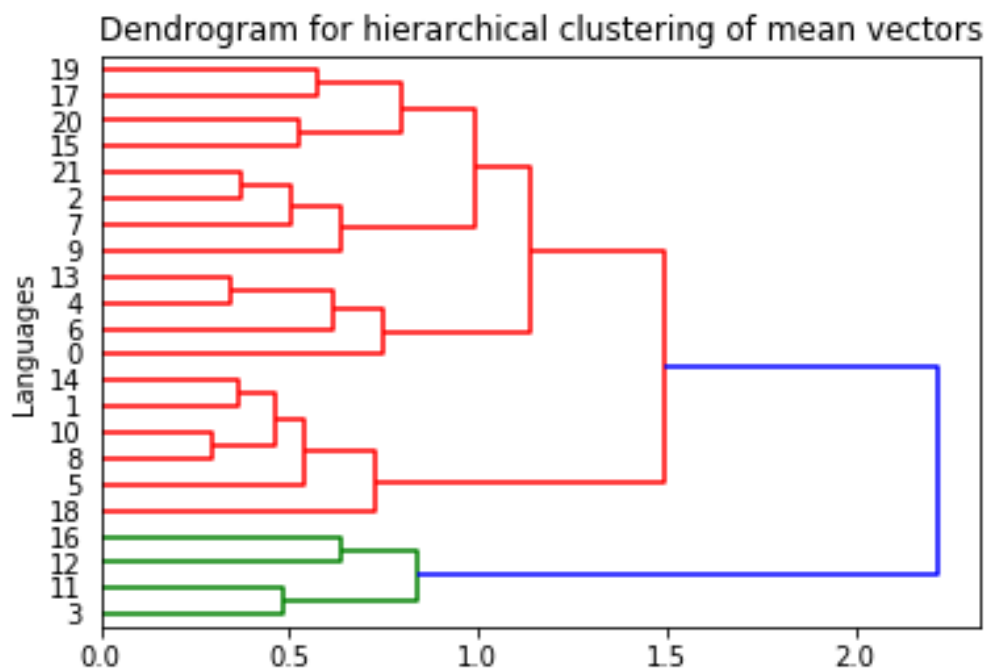
Sum of squared distances to their closest cluster centre (inertia): 38185.82.

Cluster number	Cluster size
0	1018
1	1125
2	1191
3	890
4	1162
5	1332
6	839
7	623
8	1400
9	838
10	659
11	1276
12	121
13	152
14	950
15	1971
16	1251
17	845
18	896
19	930
20	1065
21	1466

3.2 (3 points) Using the training set only, calculate the mean vector for each language, and plot the mean vectors of all the 22 languages on a 2D-PCA plane, where you apply PCA on the set of 22 mean vectors without applying standardisation. On the same figure, plot the cluster centres obtained in Question 3.1.

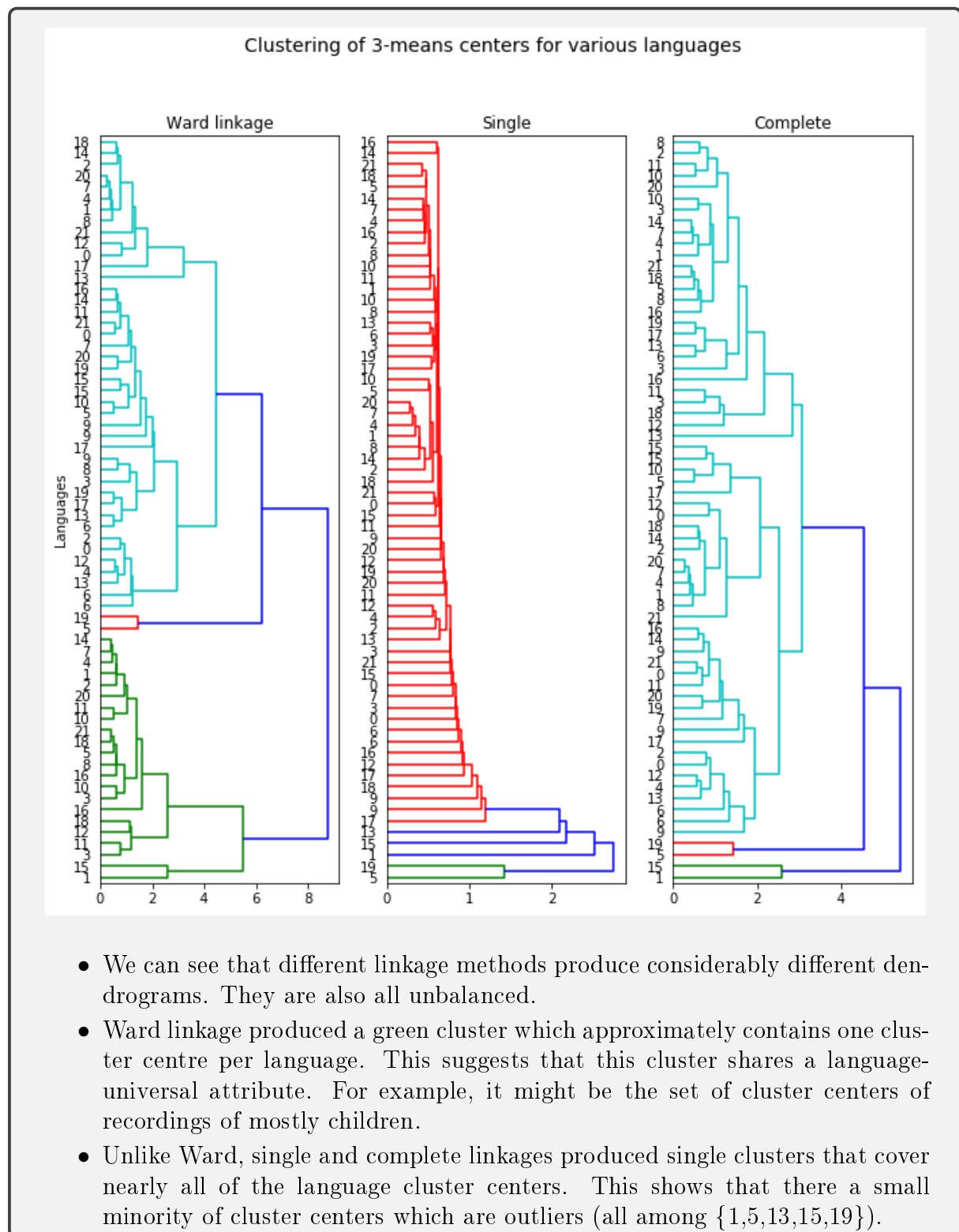


3.3 (3 points) We now apply hierarchical clustering on the training data set to see if there are any structures in the spoken languages.

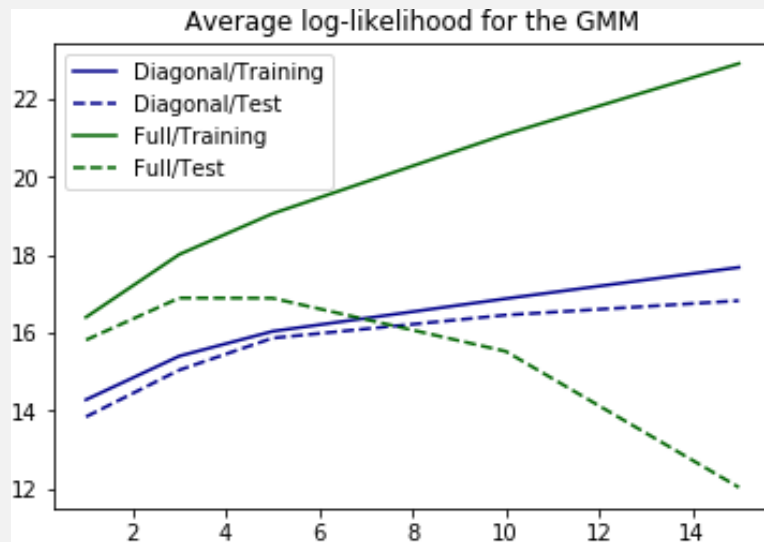


- We can see that there are 4 languages that are diametrically different from the rest ($\{3, 11, 12, 16\}$), as they are only merged with the rest in the final cluster and the distance along the final U-link is very long (represents distance here).
- More generally, we can see that the lengths of U-links do not vary too much. For example, there are no pairs of unusually similar languages.

3.4 (5 points) We here extend the hierarchical clustering done in Question 3.3 by using multiple samples from each language.



3.5 (6 points) We now consider Gaussian mixture model (GMM), whose probability distribution function (pdf) is given as a linear combination of Gaussian or normal distributions, i.e.,



	1	3	5	10	15
Diagonal/Training	14.28	15.40	16.01	16.88	17.68
Diagonal/Test	13.84	15.04	15.91	16.73	17.03
Full/Training	16.39	18.05	19.19	21.02	22.99
Full/Test	15.81	17.00	16.64	14.72	11.78

As expected, the most general model (full covariance matrix) fits the training data best. Also, this model begins to overtrain for $K > 3$. The less general model (diagonal covariance matrix) has a weaker fit, but doesn't overtrain for bigger K s.