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M1: Applied Data Science - Coursework Assignment

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Contents

1 Section A

1.1 Q1 - Dataset A

1.1.1 Question 1a

Fig(1) shows the kernel density estimates of the first 20 features of the dataset. The majority of the features are centred around 0 with little variance, except the 6 features on the bottom plot. These 6 features are likely to be more discriminative within classification algorithms, as they contain more variability.

1.1.2 Question 1b

The biplot in Fig(2) shows a PCA of the entire dataset, following standardisation. This biplot indicates that the first 20 features are no more discriminative than the rest of the features in the dataset, and the assumption that the features in Fig.(1) lower that had more variance would be more discriminative is not true as per this plot, as the green loadings tend to stretch further than the red ones. Interestingly, whilst the most discriminative features discriminate along PC2, most of the features discriminate along PC1, resulting in the large separation along PC1.

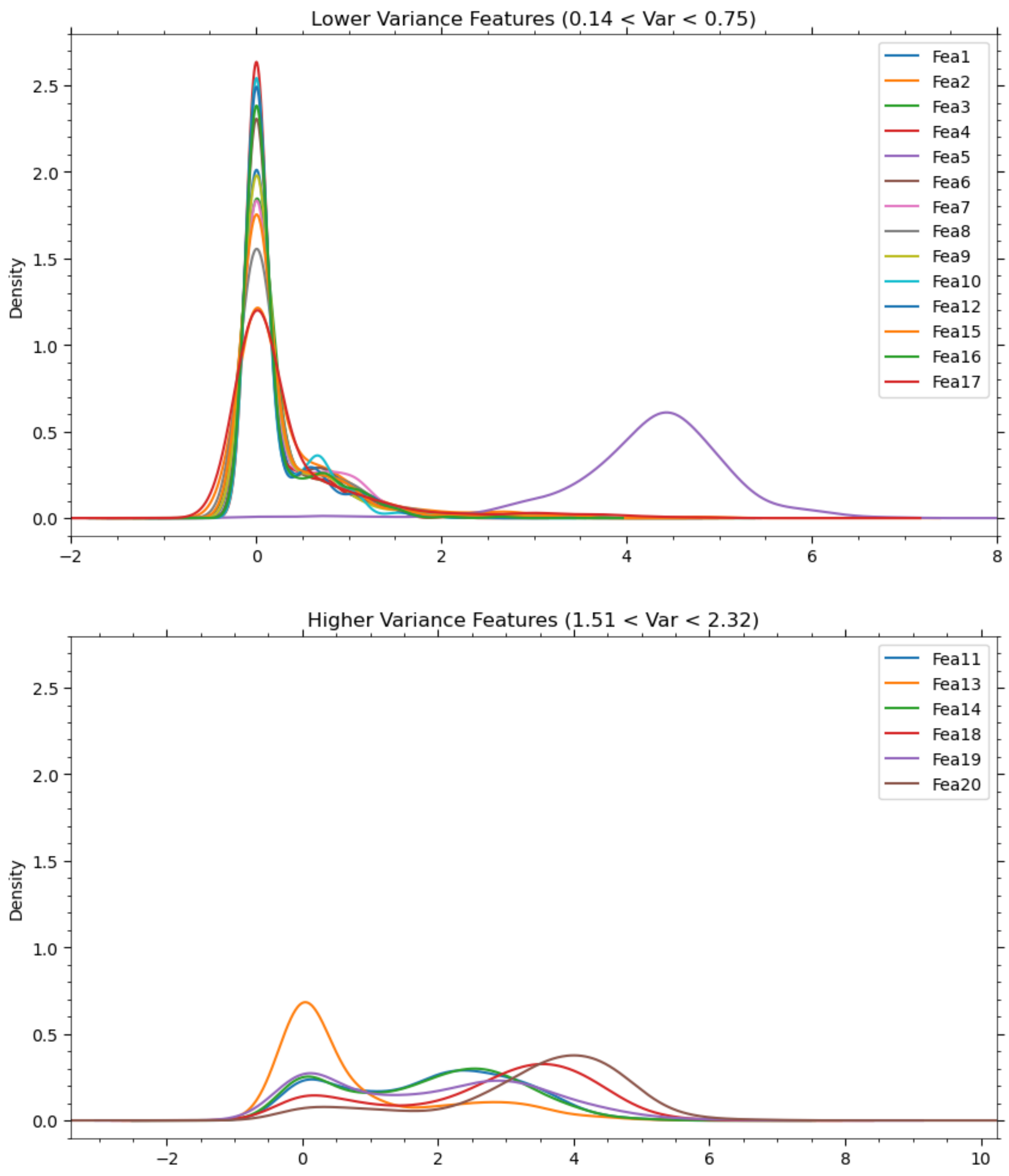


Figure 1: Kernel density estimates of the first 20 features of the `A_NoiseAdded.csv` dataset, with lower and higher variance features split into separate plots.

1.1.3 Questions 1c and 1d

Fig(3a) shows the contingency table for two k-means clusterings of the dataset with $k = 8$ and $k = 3$. Standardisation was applied before clustering as k-means is sensitive to feature scaling. The two clusterings (`kmeans_1` and `kmeans_2`) were formed by training two k-means models on half of the dataset, and then the other half were mapped onto the learned clusters by assigning new observations to the cluster whose centroid is closest to the observation [1]. This is possible because the two models were trained on the same dataset, and so the centroids are in the same feature space. Labels from each model were re-labelled using the Hungarian algorithm [2] [3] on the pair-wise distances between the centroids of each model, such that

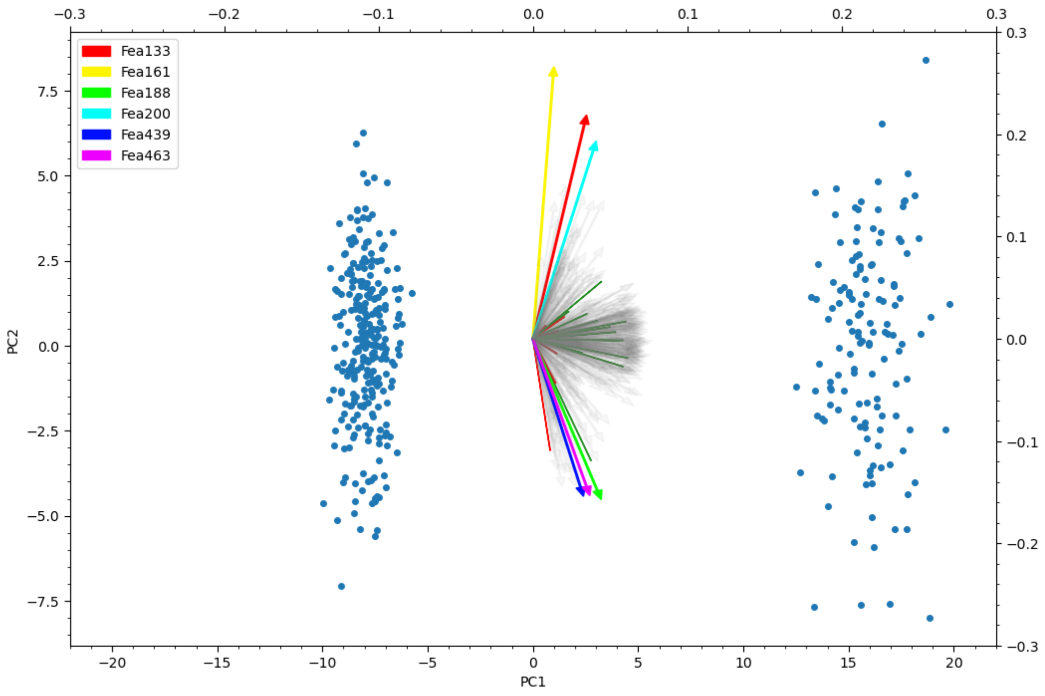


Figure 2: A biplot of the first two principal components in the `A_NoiseAdded.csv` dataset. The coloured arrows indicate the first two principal component loading vectors for every feature which contributes to either principal component more than 2%, these are the most discriminative features. Every other loading vector has been plotted in very light grey so their general directions and magnitudes are visible. The loading vectors for the Fig.(1) upper and lower have been plotted in green and red headless arrows respectively. The loading vectors use the right and top axis of the plot. The blue dots indicate the scores for each observation in the dataset for the first two principal components.

label 1 in `kmeans_1` referred to label 1 in `kmeans_2`. This step was crucial, otherwise the contingency table would be meaningless.

$k = 8$ gave a stability of 59% (the agreement on the leading diagonal), indicating that the two models were not very similar, or stable. However, `kmeans_1` clustered 85% of the observations into clusters 1, 2 and 3 and `kmeans_2` clustered 86% of the observations into clusters 1 and 2, indicates that both models correctly identified that most of the data lives within a small set of clusters. However, the presence of very small clusters indicates that there may be outliers present in the dataset or smaller clusters that the large $k = 8$ is overfitting to.

Fig(3b) shows the contingency table for two k-means clusterings of the dataset with $k = 3$, which gave a marginally better stability of 69%. A larger proportion of the observations lie on the leading diagonal compared to $k = 8$, which is expected because the number of clusters is both smaller and equal to the number of clusters in the classifications column of the dataset. `kmeans_2` identified 3 distinct clusters whereas `kmeans_1` only identified 2 distinct clusters with a few remnant observations in assigned to cluster 2.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6	Cluster 7	Cluster 8	Total
Cluster 1	**43**	0	9	8	0	4	14	1	**79**
Cluster 2	0	**185**	0	0	0	0	0	0	**185**
Cluster 3	0	87	**0**	0	0	0	0	0	**87**
Cluster 4	12	0	2	**5**	0	3	6	0	**28**
Cluster 5	1	0	0	0	**0**	0	0	0	**1**
Cluster 6	6	0	0	0	0	**0**	0	0	**6**
Cluster 7	12	0	0	0	1	1	**7**	0	**21**
Cluster 8	1	0	0	0	0	0	0	**0**	**1**
Total	**75**	**272**	**11**	**13**	**1**	**8**	**27**	**1**	**0**

(a) A contingency table for two k-means clusterings of the `A_NoiseAdded.csv` dataset, with $k = 8$, the default `scikit-learn` value. 240 of the 408 observations lie on the leading diagonal.

	Cluster 1	Cluster 2	Cluster 3	Total
Cluster 1	**155**	117	0	**272**
Cluster 2	0	**0**	10	**10**
Cluster 3	0	0	**126**	**126**
Total	**155**	**117**	**136**	**0**

(b) A contingency table for two k-means clusterings of the `A_NoiseAdded.csv` dataset, with $k = 3$. 281 of the 408 observations lie on the leading diagonal.

Figure 3: Contingency tables for two k-means clusterings of the `A_NoiseAdded.csv` dataset with number of clusters $k = 3$ and $k = 8$. Each feature in the dataset was standardised before clustering. `kmeans_1` totals are on the right and `kmeans_2` totals are on the bottom.

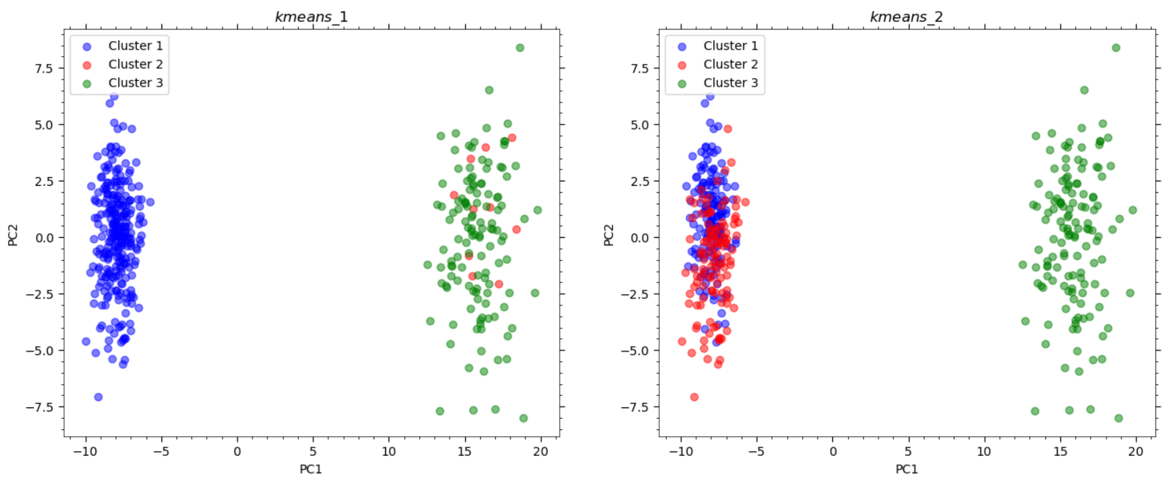


Figure 4: The k-means clusterings performed with $k = 3$, shown on the contingency table in Fig(3b), plotted on the first two principal components of the dataset shown in Fig(2).

1.1.4 Questions 1e

Fig(4) shows the k-means clusterings on the PCA plot shown in Fig(2). Visually, the 2-component PCA indicates that there are two clusters in the dataset. Fig(4) also provides subtle evidence in favour of this as well, note the instability of cluster 2 in both plots, and it's inability to capture data from both PCA groups at once. This, combined with the clear separation of clusters 1 and 3 indicate that there may only be two clusters in the dataset, as opposed to the three clusters that the labels indicate.

	Count
1	179
2	157
4	72
Missing	20
Total	**428**

(a) Raw `B_NoiseAdded.csv` dataset, before pre-processing. There are 428 observations with 20 missing labels and 20 duplicated observations (40 observations involved in the duplication).

	Count
1	177 (-3, 5, -12, 8)
2	163 (-3, 4, -5, 10)
4	68 (-4, 1, -3, 2)
Missing	0
Total	**408**

(b) `B_NoiseAdded.csv` after pre-processing, no missing labels or duplicated observations. The 4 numbers in the brackets indicate how the count in each classification changed due to, in order: 1 and 2 are counts exiting and entering (respectively) the class after correcting for mislabelling; 3 - count exiting after dropping duplicates; 4 - count entering after imputation of missing labels.

Figure 5: Summary of classifications for the `B_NoiseAdded.csv` dataset before and after pre-processing.

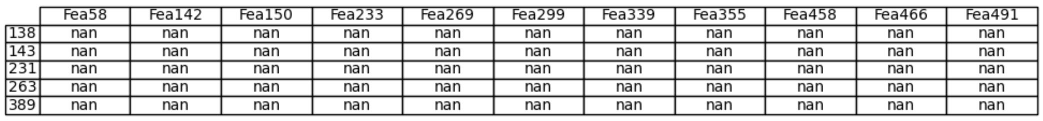
Performing k-means before PCA has the advantage of being able to visualise the clusters separation in the original feature space. However, this might not map well onto the PCA space, as the clusters may be more separable, or separate differently, in the original feature space than in the 2-component PCA space. It is generally better to perform n-component PCA (or some form of dimensionality reduction or feature selection) before k-means as it can reduce noise and mitigate the curse of dimensionality [4] where distances become less meaningful in higher dimensions.

1.2 Q2 - Dataset B

Fig.(5a) summarises the classifications for `B_NoiseAdded.csv`. The dataset contained 20 duplicates (40 involved in the duplication, full list in Appendix A) and 20 missing labels. 10 of these 20 duplicates were also mislabelled, as they contained mismatched labels across their duplicates. A multinomial `LogisticRegression` model was fit on the labelled data to predict the missing and mislabelled labels, Fig.(5b) shows the new summary of classifications.

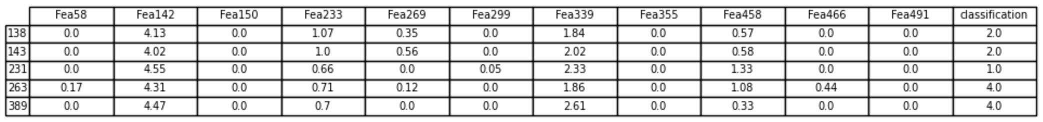
Several methods exist for handling missing labels. One method, model based imputation (used here), involves training a model on labelled data to predict missing labels. Alternatively, data with missing labels can be ignored, especially if the sample size is large. Whilst model based imputation utilises all data, it risks bias if the model poorly fits the data. Ignoring missing data avoids bias, if the samples size is large.

Missing at random (MAR) means a label's absence is unrelated to its value, whereas missing not at random (MNAR) indicates a correlation between a label's absence and its value. In Fig.(5b), the missing labels' percentages in each class (4.5%, 6.1%, and 2.9% for



	Fea58	Fea142	Fea150	Fea233	Fea269	Fea299	Fea339	Fea355	Fea458	Fea466	Fea491
138	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
143	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
231	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
263	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
389	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan

(a) The samples and features with missing data.



	Fea58	Fea142	Fea150	Fea233	Fea269	Fea299	Fea339	Fea355	Fea458	Fea466	Fea491	classification
138	0.0	4.13	0.0	1.07	0.35	0.0	1.84	0.0	0.57	0.0	0.0	2.0
143	0.0	4.02	0.0	1.0	0.56	0.0	2.02	0.0	0.58	0.0	0.0	2.0
231	0.0	4.55	0.0	0.66	0.0	0.05	2.33	0.0	1.33	0.0	0.0	1.0
263	0.17	4.31	0.0	0.71	0.12	0.0	1.86	0.0	1.08	0.44	0.0	4.0
389	0.0	4.47	0.0	0.7	0.0	0.0	2.61	0.0	0.33	0.0	0.0	4.0

(b) The imputed data.

Figure 6: Samples and features with missing data, for the `C_MissingData.csv` dataset.

classes 1, 2, and 4) suggest no significant evidence of MNAR.

1.3 Q3 - Dataset C

1.3.1 Questions 3a and 3b

Figure (6a) displays features with missing values and corresponding samples. Several methods address missing data. Static imputation, a simple approach, replaces missing values in a feature with a constant value, like the feature's mean. Although computationally cost-effective, it may decrease variance and bias datasets with many missing values. Alternatively, model based imputation estimates missing values per sample using a suitable model. For example, the K Nearest Neighbours method imputes a feature's missing value using the mean of that value from the sample's K nearest neighbours. This approach can mitigate bias and maintain variance, but in high-dimensional data, it may lead to less meaningful nearest neighbours, as distances become less meaningful with increased dimensions [4].

Multiple imputation involves using a probabilistic model to impute missing data several times, creating multiple datasets. These datasets can be analysed individually or their imputed values averaged. This method captures uncertainty in missing data, and is particularly useful when missing data is extensive.

1.3.2 Question 3c

Fig(7) depicts a simulation where data was removed and re-imputed using PCA and KNN to assess imputation accuracy at different `n_neighbors` values. This helped in selecting `n_neighbors=15` for KNN imputation, as larger `n_neighbors` values did not significantly improve accuracy (lower MSE). KNN combined with PCA mitigates the 'curse of dimensionality,' improving accuracy [4] and aiding in identifying more meaningful neighbours. KNN is preferable for clustered datasets where distance-based methods are effective and it is expected that nearest neighbours share similar properties.

Fig(6b) displays the data imputed with PCA and KNN. Fig(8) indicates that this method largely preserved the original feature distributions.

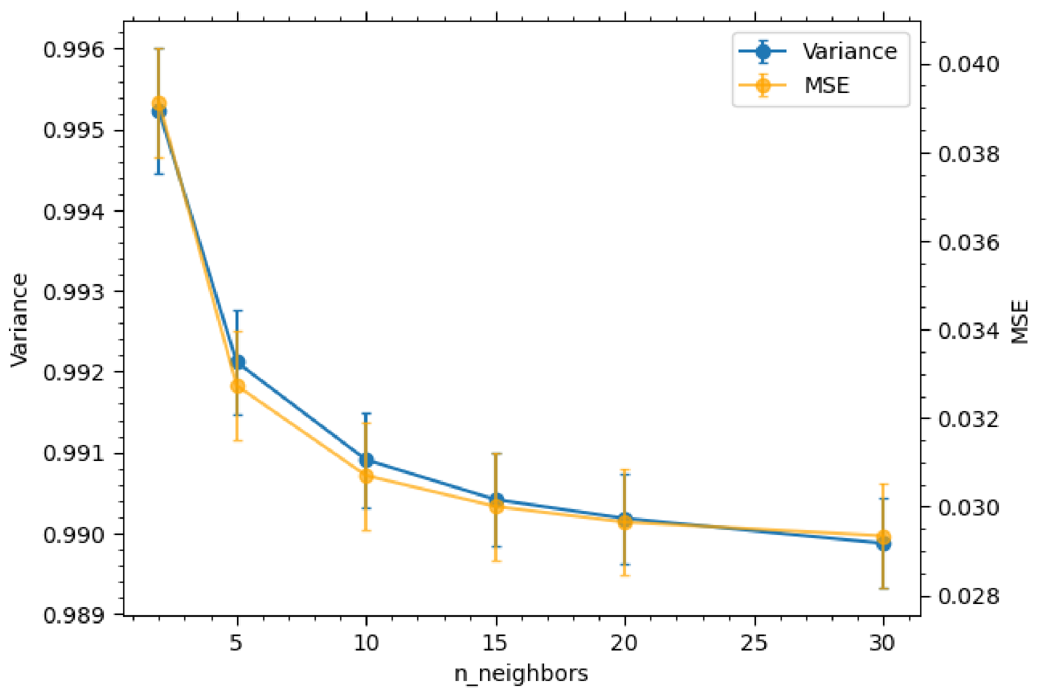
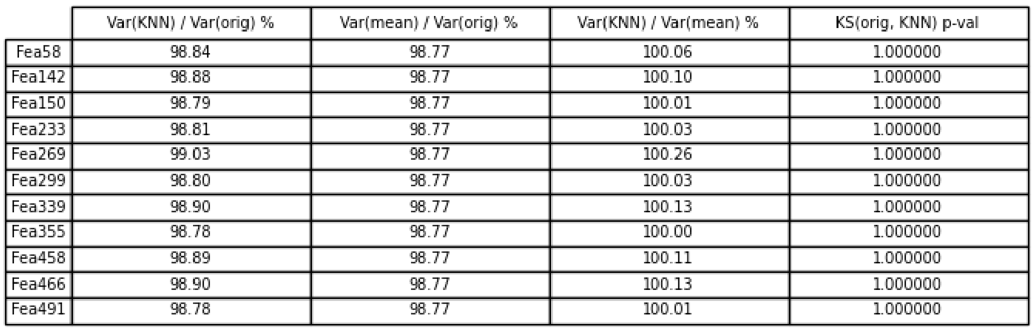


Figure 7: Variance and MSE of KNN imputed data, for different values of `n_neighbors`. The variance is shown as a percentage of the original dataset, and the MSE is the mean squared error of predicted values against the true values.



	Var(KNN) / Var(orig) %	Var(mean) / Var(orig) %	Var(KNN) / Var(mean) %	KS(orig, KNN) p-val
Fea58	98.84	98.77	100.06	1.000000
Fea142	98.88	98.77	100.10	1.000000
Fea150	98.79	98.77	100.01	1.000000
Fea233	98.81	98.77	100.03	1.000000
Fea269	99.03	98.77	100.26	1.000000
Fea299	98.80	98.77	100.03	1.000000
Fea339	98.90	98.77	100.13	1.000000
Fea355	98.78	98.77	100.00	1.000000
Fea458	98.89	98.77	100.11	1.000000
Fea466	98.90	98.77	100.13	1.000000
Fea491	98.78	98.77	100.01	1.000000

Figure 8: This table compares feature variances post-imputation. Column 1 displays each feature's variance after KNN imputation, as a percentage of the original dataset. Column 2 does the same for mean imputation. Column 3 contrasts the values from columns 1 and 2. Column 4 presents the p-value from the Kolmogorov-Smirnov test, comparing the original and KNN imputed datasets.

1.3.3 Question 3d and 3e

Outliers were identified by standardising the data and identifying values over 3σ from the mean. Fig(9) indicates uniformly distributed outliers across the dataset.

These outliers were imputed using PCA and KNN, similar to Question 3c, with the

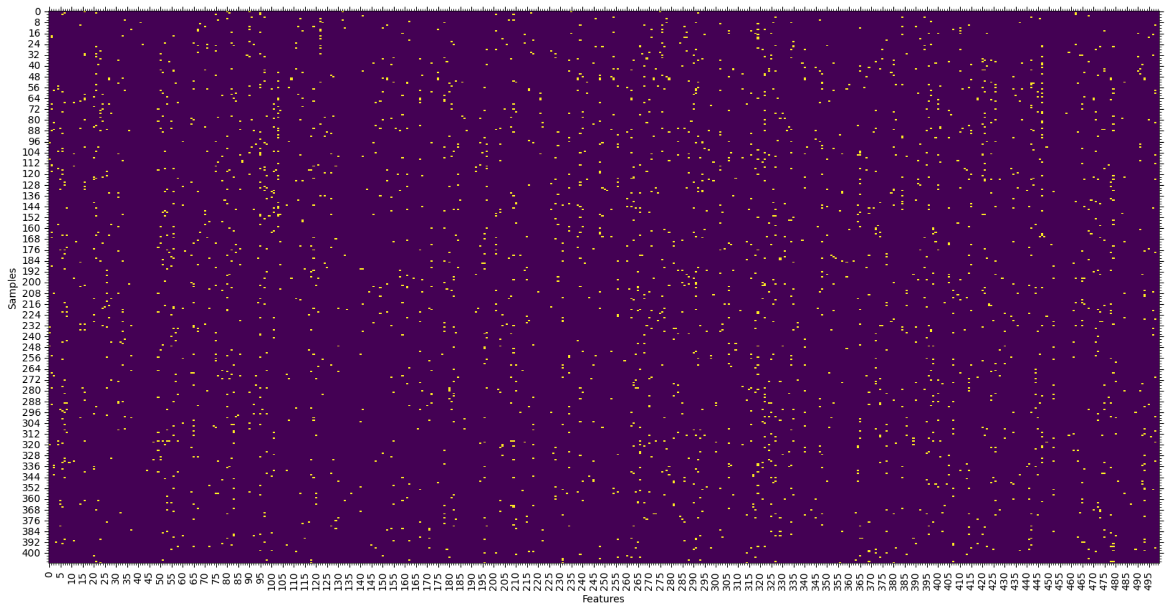


Figure 9: A heatmap of the outliers in the `C_MissingFeatures.csv` dataset. The orange marks indicate an outlier value, 2904 outlier values were identified.

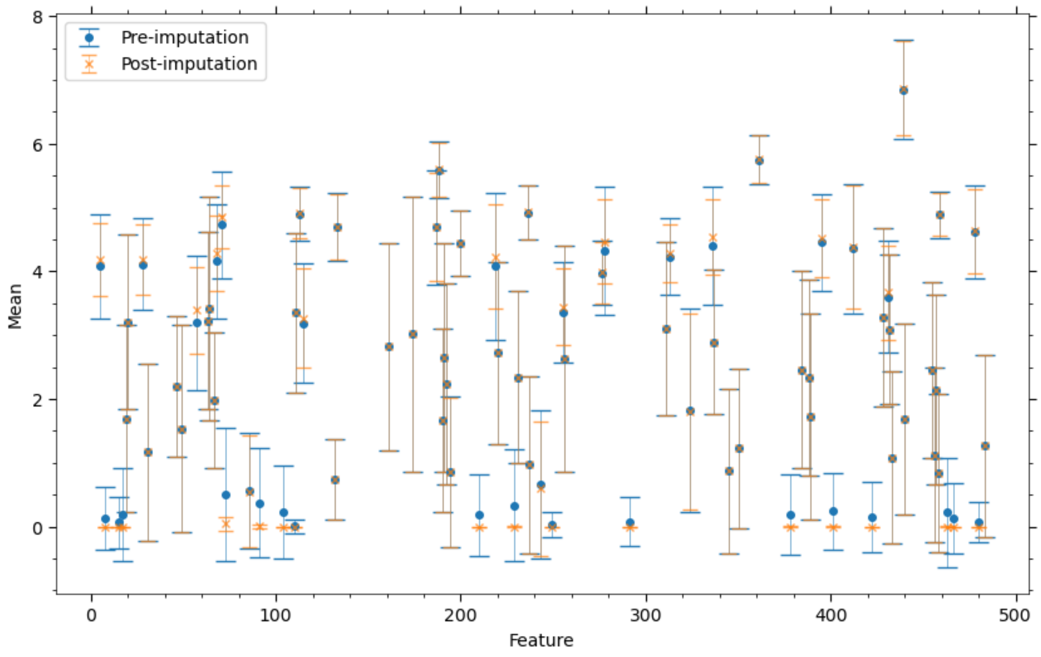


Figure 10: The mean and standard deviation of the 81 most discriminative features in the original `C_MissingFeatures.csv` dataset, before and after outlier imputation.

justification being identical to Question 3c. Outliers were iteratively removed, with re-standardisation and outlier detection after each iteration. The process iterated 8 times, stopping after only 0.27% of the samples were outside 3σ, aligning with normal distribution expectations.

Fig(10) compares the mean and standard deviation of the 81 most discriminative features, before and after outlier imputation. Feature variance decreased post-imputation (as expected), more so for features with near-zero means, likely due to their sparsity and higher outlier likelihood.

2 Section B

2.1 Q4 - Baseline Dataset

2.1.1 Question 4a

Classification decision trees utilise recursive binary splitting to split the feature-space into high dimensional rectangles in order to predict the outcome class given a feature set. In each iteration, an existing rectangle is split into two new rectangles, by splitting on a feature and a threshold value for that feature. The end tree will have some number of internal nodes N_n, representing splits in the feature space, and $N_n + 1$ terminal nodes which represent the final classification, which would be the modal class in that rectangle. The quality of the split can be measured by a criterion such as the Gini index, and at each split, the feature to split on and the threshold would be chosen by whichever split decreases the Gini index the most. The Gini index is defined as [5]:

$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \tag{2.1}$$

where $\hat{p}_{mk}$ is the proportion of training samples in the mth region that are from the kth class. A region m that contains mainly a single class will have a small Gini index for that region.

Decision trees suffer from high variance as the trained model is highly dependent on the training data. Bagging and random forests are ensemble methods that reduce the variance of decision trees. With bagging, multiple decision trees are trained on different bootstrapped samples of the training data, and the classification is then decided by a majority vote of the trees. Random forests reduce the variance further by forcing an internal node to split on a random subset of the features, resulting in less correlated trees, and therefore a larger decrease in variance.

Two hyperparameters of random forests `max_depth` and `max_features`, the former is the maximum number of internal nodes per tree, and the latter is the number of features to consider when splitting. Heuristically, `max_depth` is typically set to $\sqrt{N}$ where N is the number of features.

2.1.2 Question 4b, 4c, 4d and 4e

The dataset was pre-processed using the same outlier removal technique as in Section 1.3.3, and then standardised. No duplicates or missing values were found. The dataset contained imbalanced classes, as such, stratified sampling was used for train-test splitting.

The dataset was then classified using `RandomForestClassifier` and Fig.(11) shows a summary of the model performance, averaged over 5-folds of cross validation. This gave a test set classification error of 11%.

The `RandomForestClassifier` was then optimised using the out-of-bag (OOB) error rate, the results of this is shown in Fig. (12) where it was found that after 200 trees, the OOB error rate did not decrease by any significant amount. Fig. (13) shows the summary of the model performance with 200 trees. The test set classification error marginally improved to

	1	2	3	Tot. (actual)
1	**0.372**	0.002	0.006	0.38
2	0.016	**0.334**	0.006	0.356
3	0.056	0.014	**0.194**	0.264
Tot. (predictions)	0.444	0.35	0.206	

(a) Mean confusion matrix.

	Precision	Recall	F1-score	True count
1	0.839	0.979	0.903	38.0
2	0.955	0.938	0.946	36.0
3	0.942	0.734	0.824	26.0
Macro Avg	0.912	0.884	0.891	
Weighted Avg	0.907	0.9	0.898	

(b) Mean classification report.

Figure 11: Confusion matrix and classification report averaged over 5-folds of cross validation for the random forest classifier on `ADS_baselineDataset.csv`. The leading diagonal of the confusion matrix indicates a mean 10.0% test set classification error. The confusion matrix cells are shown as percentages of the total number of samples in the test set. The train test split was 0.8/0.2, giving a test set size of 100.

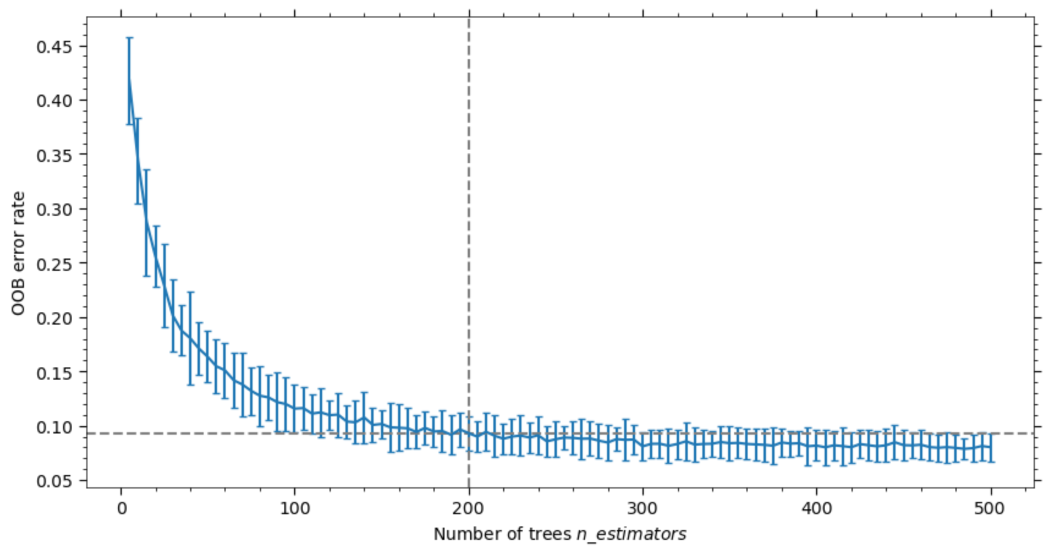


Figure 12: The out of bag error rate for a `RandomForestClassifier` on the pre-processed dataset `ADS_baselineDataset.csv`. The OOB error rate was computed 20 times at each value of `n_estimators` to give error bars.

	1	2	3	Tot. (actual)
1	**0.372**	0.0	0.008	0.38
2	0.012	**0.338**	0.006	0.356
3	0.048	0.012	**0.204**	0.264
Tot. (predictions)	0.432	0.35	0.218	

(a) Mean confusion matrix.

	Precision	Recall	F1-score	True count
1	0.862	0.979	0.916	38.0
2	0.966	0.949	0.957	36.0
3	0.939	0.772	0.845	26.0
Macro Avg	0.922	0.9	0.906	
Weighted Avg	0.919	0.914	0.912	

(b) Mean classification report.

Figure 13: The results shown in Fig. (11) but with 200 trees. The mean test set classification error was 8.6%.

9% and the average precision, recall and F1-scores also marginally improved. These results are in line with Fig. (12) which shoes a noticeable but not significant decrease in the OOB error rate from 100 to 200 trees.

The feature importance was then computed using the Gini importance given within `RandomForestClassifier.feature_importances_` as shown in Fig. (14). The Gini

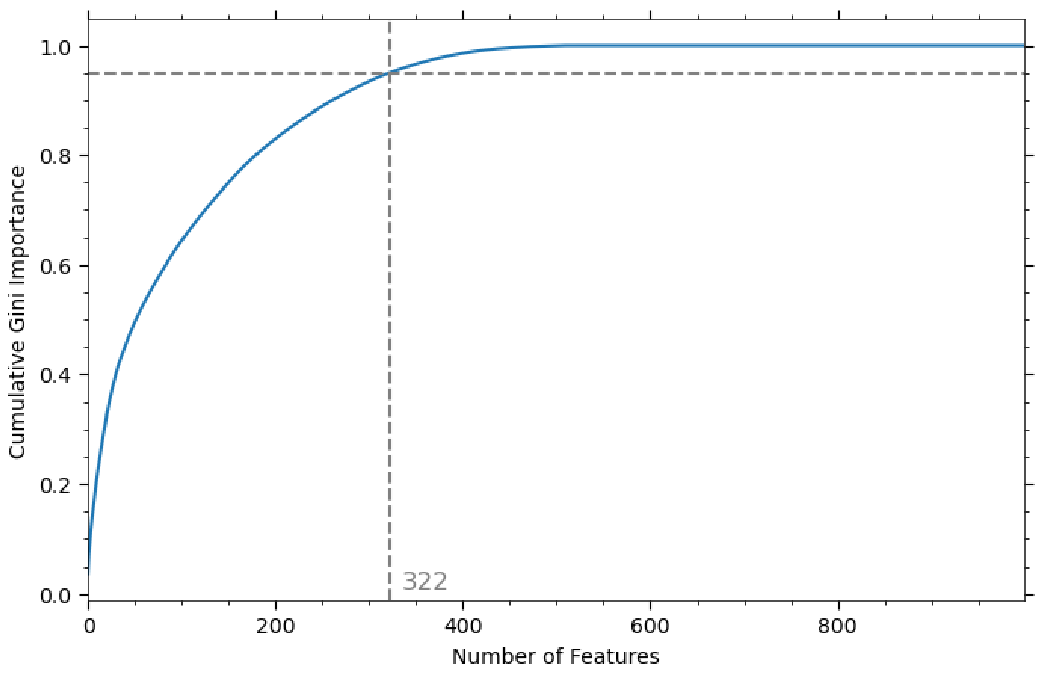
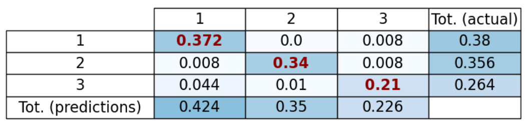
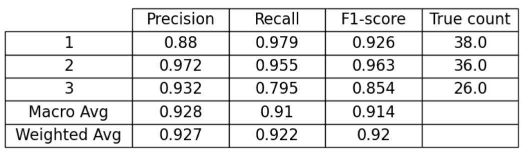


Figure 14: The ordered (highest first), cumulative Gini importance of the features in `ADS_baselineDataset.csv`. The horizontal grey line is the 95% threshold, which contains the top 322 features.



	1	2	3	Tot. (actual)
1	**0.372**	0.0	0.008	0.38
2	0.008	**0.34**	0.008	0.356
3	0.044	0.01	**0.21**	0.264
Tot. (predictions)	0.424	0.35	0.226	

(a) Mean confusion matrix.



	Precision	Recall	F1-score	True count
1	0.88	0.979	0.926	38.0
2	0.972	0.955	0.963	36.0
3	0.932	0.795	0.854	26.0
Macro Avg	0.928	0.91	0.914	
Weighted Avg	0.927	0.922	0.92	

(b) Mean classification report.

Figure 15: The results shown in Fig. (11) and Fig. (13) but with 200 trees and utilising only the top 322 features. The mean test set classification error was 7.8%.

importance of a feature is defined as the total (normalised) decrease in the Gini index as a result of all internal splits within trees that split on a given feature, so a feature is more important if it is used in many splits, and if these splits consequently result in a large decrease in the Gini index. The top 322 features containing 95% of the cumulative Gini importance were then selected to redo the classification, and the results are shown in Fig.(15). Fig.(15), when compared to Fig.(13), shows that equivalent (or marginally better) performance is achievable by only using the subset of most important features.

2.1.3 Question 4f

Everything in the previous section, Sec.(2.1.2), was then repeated for a multinomial logistic regression classifier: `LogisticRegression`. Fig.(16) shows the results of the classification using all features, and Fig.(17) shows the results of the classification using only the top 382 features, which shows a significant increase in performance in terms of test set classification error and average precision, recall and F1-scores. The feature importance was computed

	1	2	3	Tot. (actual)
1	**0.33**	0.014	0.036	0.38
2	0.018	**0.328**	0.01	0.356
3	0.036	0.014	**0.214**	0.264
Tot. (predictions)	0.384	0.356	0.26	

(a) Mean confusion matrix.

	Precision	Recall	F1-score	True count
1	0.865	0.868	0.864	38.0
2	0.923	0.921	0.921	36.0
3	0.821	0.81	0.813	26.0
Macro Avg	0.869	0.867	0.866	
Weighted Avg	0.874	0.872	0.871	

(b) Mean classification report.

Figure 16: Confusion matrix and classification report averaged over 5-folds of cross validation for the `LogisticRegression` classifier on `ADS_baselineDataset.csv`. The leading diagonal of the confusion matrix indicates a mean 12.8% test set classification error. The confusion matrix cells are shown as percentages of the total number of samples in the test set. The train test split was 0.8/0.2, giving a test set size of 100.

	1	2	3	Tot. (actual)
1	**0.354**	0.008	0.018	0.38
2	0.014	**0.334**	0.008	0.356
3	0.016	0.012	**0.236**	0.264
Tot. (predictions)	0.384	0.354	0.262	

(a) Mean confusion matrix.

	Precision	Recall	F1-score	True count
1	0.923	0.932	0.927	38.0
2	0.944	0.938	0.941	36.0
3	0.901	0.894	0.896	26.0
Macro Avg	0.923	0.921	0.921	
Weighted Avg	0.925	0.924	0.924	

(b) Mean classification report.

Figure 17: The results shown in Fig. (16) but with only the top 382 features. The mean test set classification error was 7.6%.

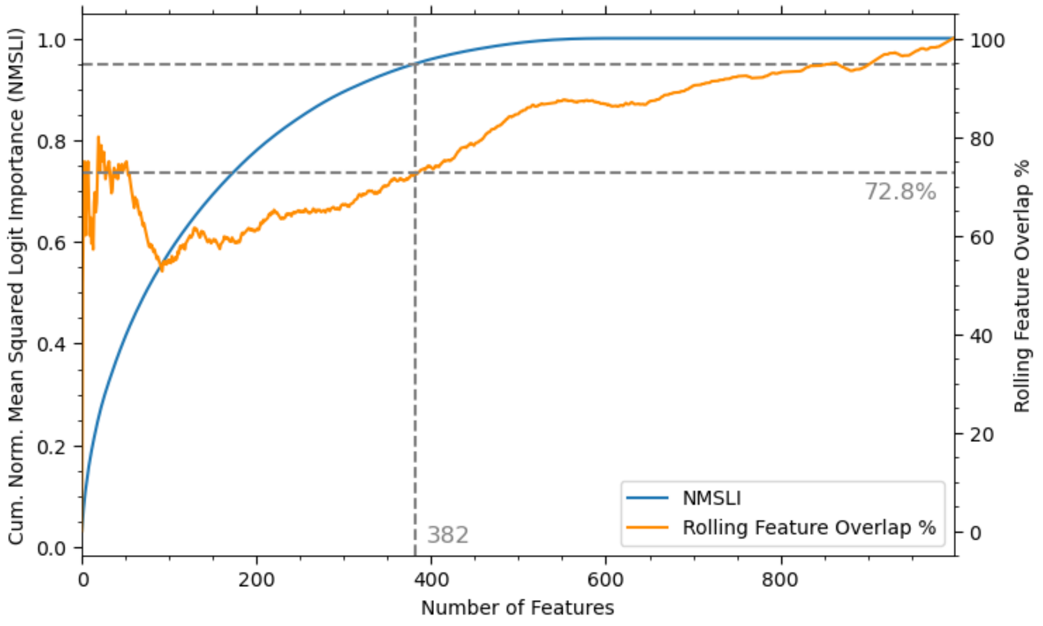


Figure 18: The ordered (highest first), cumulative NMSLI of the features in the `LogisticRegression` model. The horizontal grey line is the 95% threshold, which contains the top 382 features. Amongst the 382 top features indicated by the NMSLI, 72.8% of them were also in the top 382 features for the `RandomForestClassifier` indicated by the Gini importance, this is what the rolling feature overlap indicates.

using a novel metric, the normalised mean squared logit importance (NMSLI). This was computed by averaging the squared coefficients across all 3 classes for each feature (by accessing `LogisticRegression.coef_`) and then normalising them. This provided a feature-wise metric for importance, akin to the Gini importance, which took into account the magnitude and consistency of the coefficients across all classes. This was then treated the same as the Gini importance, giving the top 382 features which contributed to 95% of the cumulative NMSLI, as shown in Fig.(18). Comparing Fig.(15) and Fig.(17), both models performed very similarly across all metrics.

2.2 Q5 - Baseline Dataset

2.2.1 Question 5a

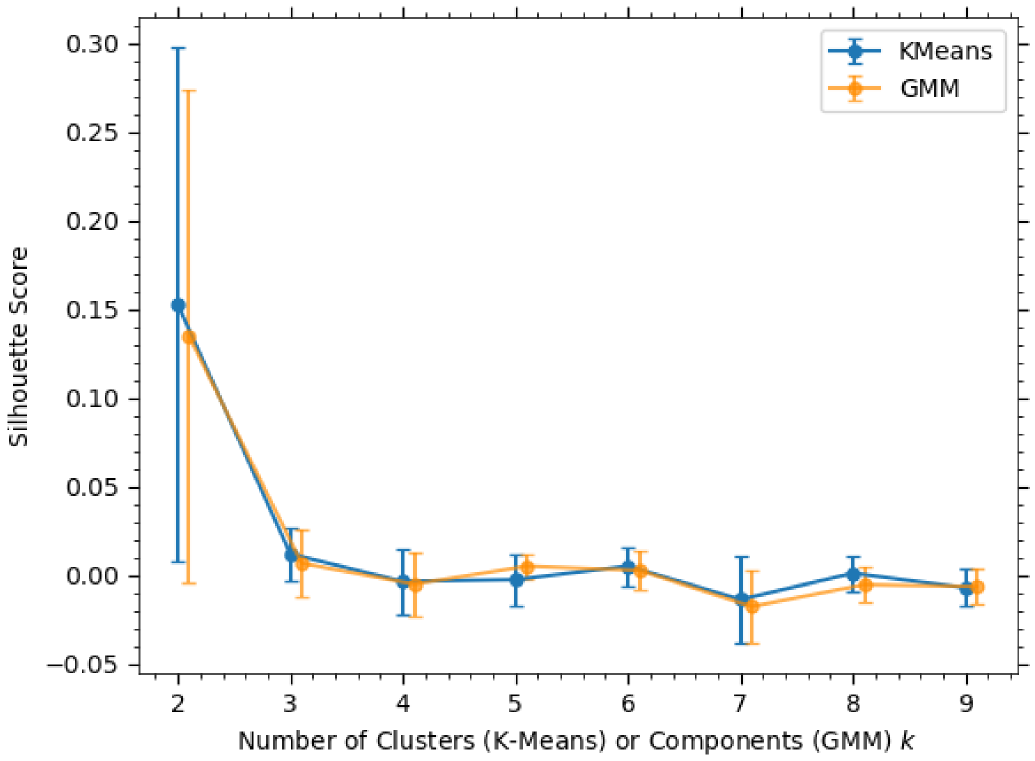


Figure 19: The silhouette scores for the K-Means and Gaussian Mixture Models on the pre-processed `ADS_baselineDataset.csv` dataset. 5 repetitions were performed to give a mean and standard deviation for each k value.

The dataset `ADS_baselineDataset.csv` was pre-processed in the same way as it was for Q4 and Q3e, and then K-Means and Gaussian Mixture Models were applied to the dataset. The `KMeans` implementation used utilised the Lloyd's algorithm which yields k centroids with each sample being assigned to the nearest centroid, this works under the assumption that the data is generally spherically distributed. The `GaussianMixture` implementation used utilised the expectation-maximisation algorithm which yields k Gaussian distributions with each sample being assigned to the distribution with the highest probability, this works under the assumption that the data is generated by a mixture of Gaussian distributions, so can be a bit more flexible than K-Means.

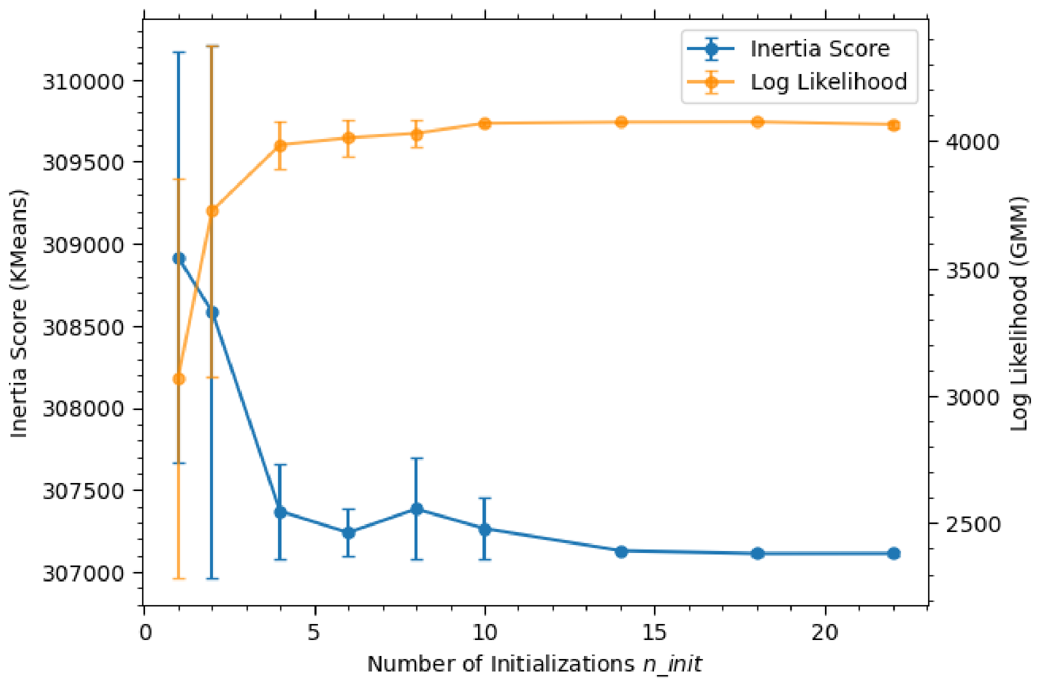
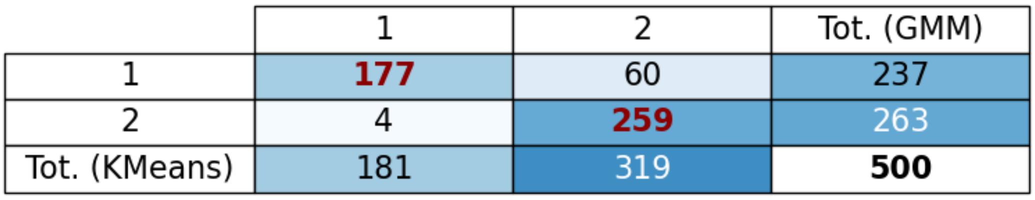


Figure 20: The score of the cost functions for the K-Means and Gaussian Mixture Models as `n_init` is increased 5 repetitions were performed to give a mean and standard deviation for each `n_init` value.



	1	2	Tot. (GMM)
1	**177**	60	237
2	4	**259**	263
Tot. (KMeans)	181	319	**500**

Figure 21: A contingency table comparing cluster assignments for the K-Means and Gaussian Mixture Models on the pre-processed `ADS_baselineDataset.csv` dataset, with $k = 2$ and $n\_init = 50$. The leading diagonal gives an 87.2% agreement between the two models.

Fig. 19 shows the silhouette scores for the K-Means and Gaussian Mixture Models on the data, indicating that the optimal number of clusters was $k = 2$ for both algorithms. However, the large errors on $k = 2$ indicated large instability in the algorithms ability to find a global minima, as such, Fig. 20 shows the effect of increasing the number of initialisations on the cost function for both algorithms. Both algorithms are very dependent on the random initialisation of the centroids/distributions and the dissappearance of the error bars on both models at $n\_init > 10$ indicated that the algorithms required at leeast this many random initialisations to find a global minima. Therefore, $n\_init = 50$ was used hereon.

Fig. 21 shows a contingency table comparing the cluster assignments for the K-Means and Gaussian Mixture Models using these parameters, 87.2% agreement was found.

2.2.2 Question 5b

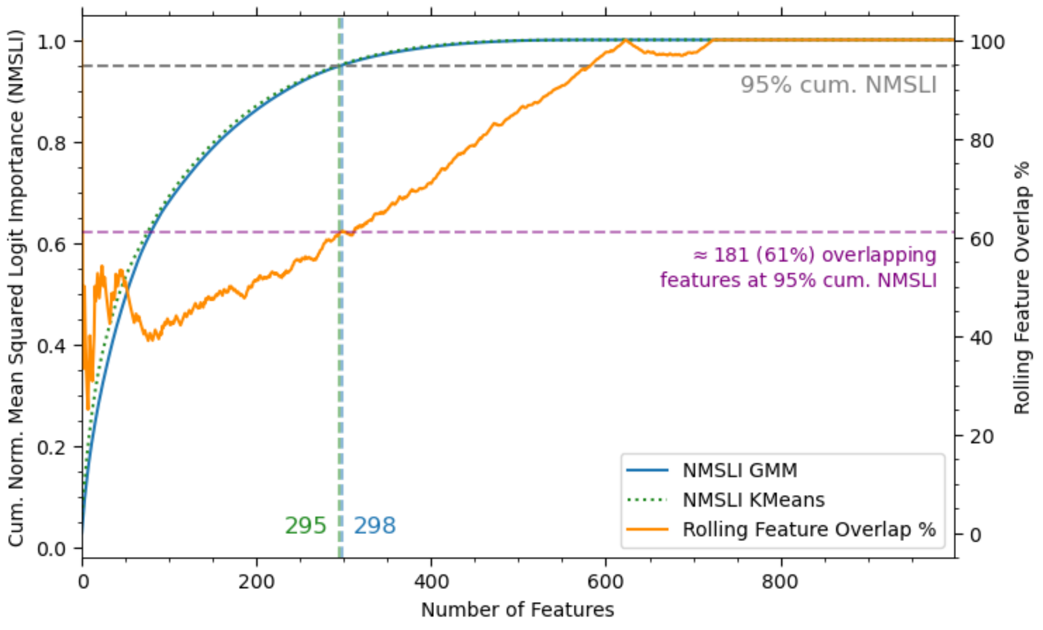
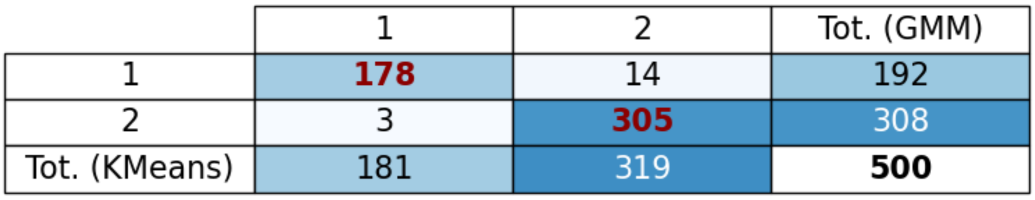


Figure 22: The feature importance for the K-Means and Gaussian Mixture Models using a `LogisticRegression` classifier and the NMSLI metric on the classified data shown in Fig. (21). The 95% NMSLI threshold selected 295 and 298 important features for K-means and GMM respectively, and the orange line indicates that roughly 181 of these features were shared between the two models.



	1	2	Tot. (GMM)
1	**178**	14	192
2	3	**305**	308
Tot. (KMeans)	181	319	**500**

Figure 23: A contingency table comparing cluster assignments for the K-Means and Gaussian Mixture Models after feature reduction as shown in Fig. (22). The leading diagonal shows a 96.6% agreement between the two models.

A `LogisticRegression` classifier was utilised on the classified data shown in Fig. (21) to determine the feature importance, as shown in Fig. (22), using the NMSLI metric (derived and explained in Section (2.1.3)). The top 295 and 298 important features for K-means and GMM respectively were utilised to train a new K-Means and Gaussian Mixture Model, as shown in Fig. (23), 96.6% agreement was found, a significant improvement over the 87.2% agreement found in Fig. (21).

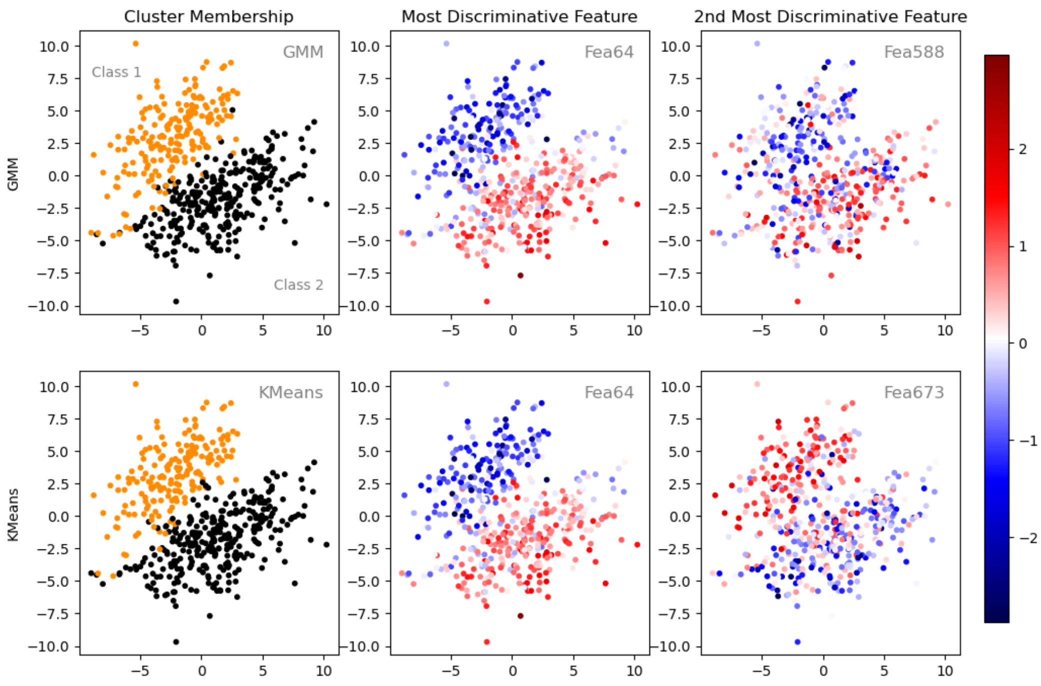


Figure 24: PCA visualisations of the clusters found by the K-Means and Gaussian Mixture Models as shown in Fig. (23). The top row is for the K-Means model and the bottom row is for the GMM. The left column shows the cluster membership, the middle and right columns show the samples coloured by the first and second most important discriminative respectively. The x-axis is the first principal component and the y-axis is the second principal component for all plots.

2.2.3 Question 5c

Fig. (24) shows the PCA visualisations of the clusters found by the K-Means and Gaussian Mixture Models. The middle column indicates a strong positive correlation along $y = -x$ for the most discriminative feature (which was the same for both models), and the right column indicates a slightly weaker but still existent positive correlation along the same line for the second most discriminative feature (which was different for both models).

A Q2: Duplicate Observations in `B_NoiseAdded.csv`

The duplicated pairs in `B_NoiseAdded.csv`, the number is the sample number: [[74 146], [220 291], [147 409], [44 193], [66 253], [28 260], [384 396], [188 249], [83 198], [175 311], [166 424] [344 389], [117 297], [351 352], [120 359], [119 382], [100 173], [30 101], [46 107], [210 305]]

References

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