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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 lower plot. Values range from 0 to roughly 7. The lower variance data centred around mean 0 tend to have more leptokurtic distributions with slightly positive skew indicating higher likelihood of outliers being present, whilst the higher variance data is more platykurtic with less skew.

1.1.2 Question 1b

The biplot in Fig.(2) shows a PCA of the entire dataset, following standardisation. The discriminative power of the first 20 features is average, and the higher variance features in Fig.(1) are not, on average, any more discriminative than the lower variance features. Interestingly, whilst the most discriminative features discriminate along PC2, most of the features discriminate along PC1, resulting in the large separation along PC1.

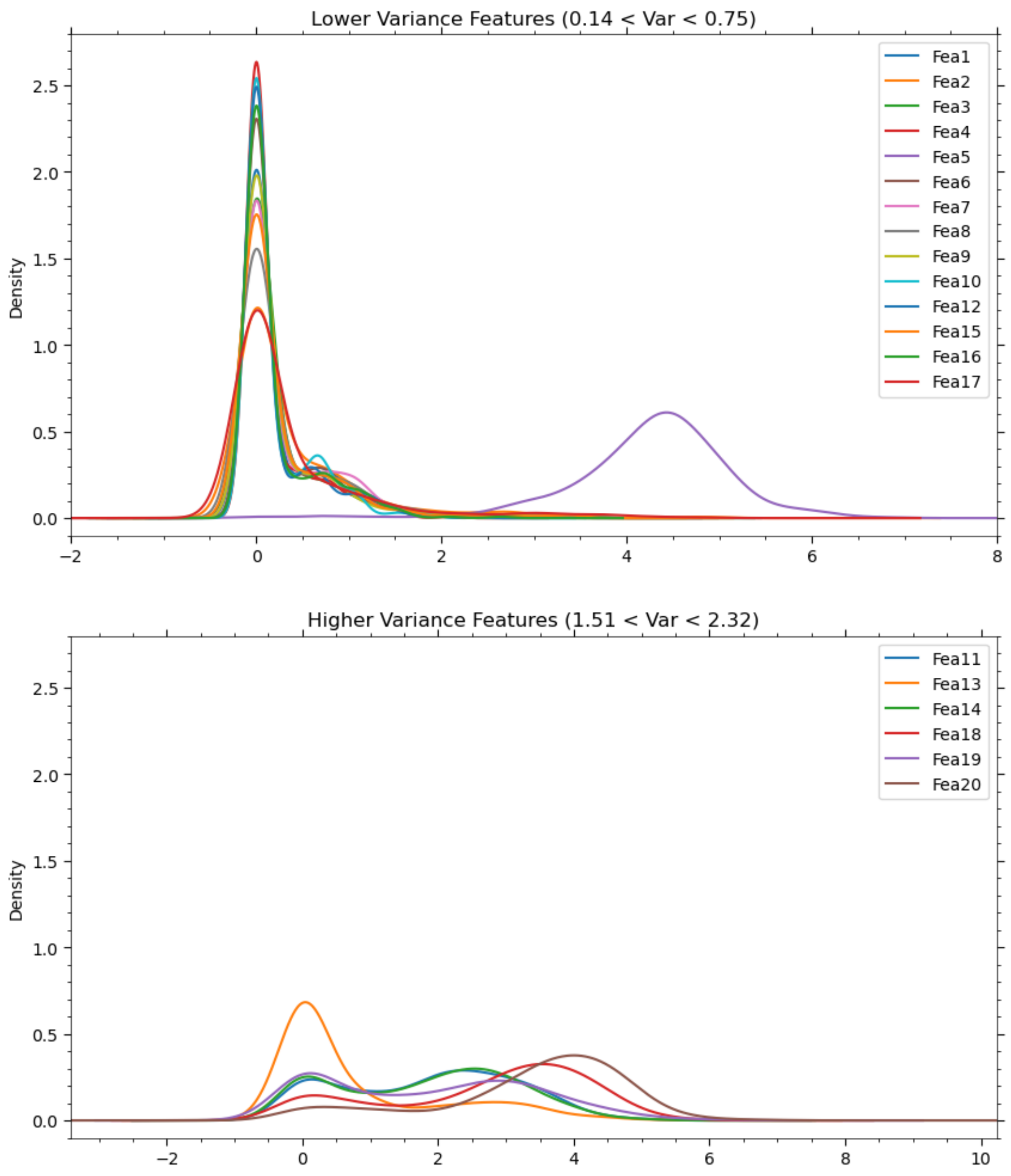


Figure 1: Kernel density estimates of the first 20 features of the `A_NoiseAdded.csv` dataset, with lower and higher variance features split into separate plots.

1.1.3 Questions 1c and 1d

Fig.(3) 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 was 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 defined 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,

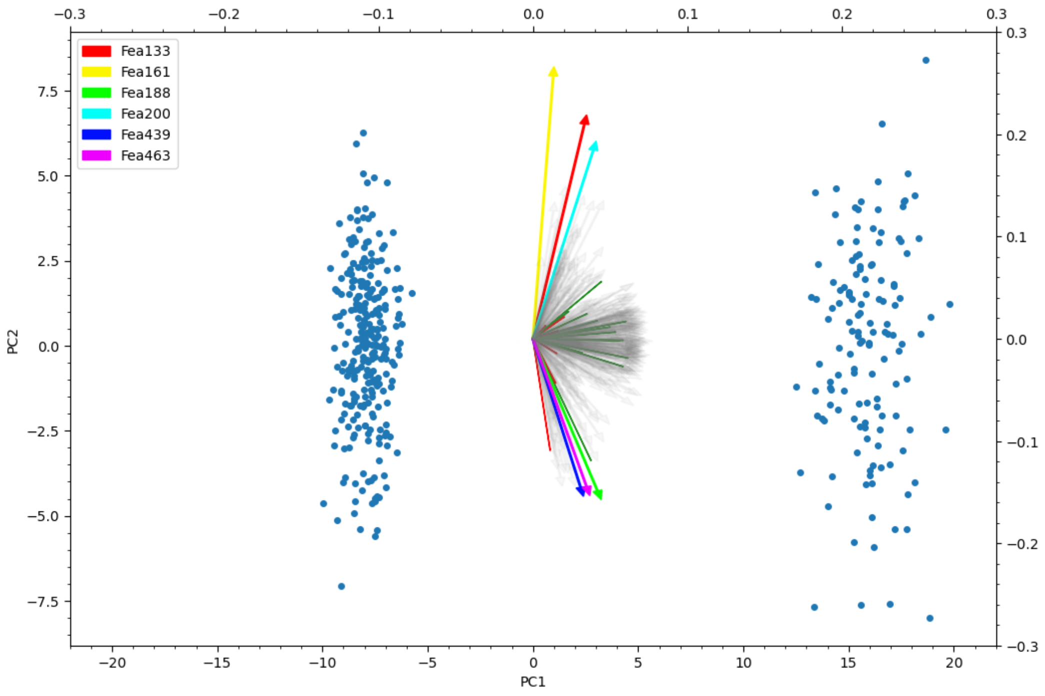


Figure 2: A biplot of the first two principal components in the `A_NoiseAdded.csv` dataset. The coloured arrows indicate the first two principal component loading vectors for every feature which contributes to either principal component more than 2%, these are the most discriminative features. Every 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.

such that label 1 in `kmeans_1` referred to label 1 in `kmeans_2`, and so on. This step was crucial, otherwise the contingency tables would be meaningless.

$k = 8$ gave a stability of 59%, 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, indicating 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 was 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. So both models ($k = 8$ and $k = 2$) identified a similar number of distinct clusters to which most of the samples belonged to.

	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**	

(a) A contingency table for two k-means clusterings of the `A_NoiseAdded.csv` dataset, with $k = 8$, the default `scikit-learn` value. 240 (59%) 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**	

(b) A contingency table for two k-means clusterings of the `A_NoiseAdded.csv` dataset, with $k = 3$. 281 (69%) 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.

1.1.4 Questions 1e

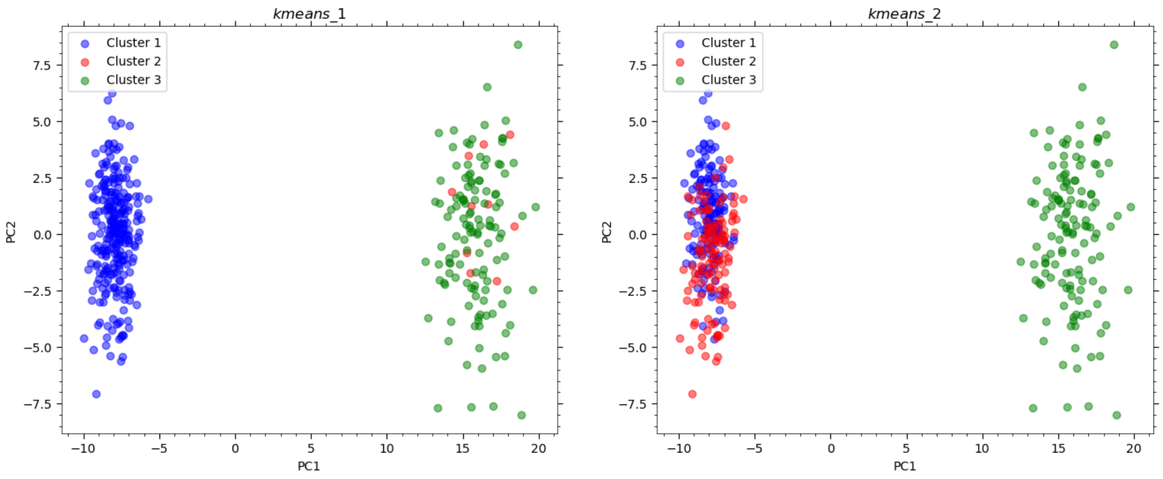
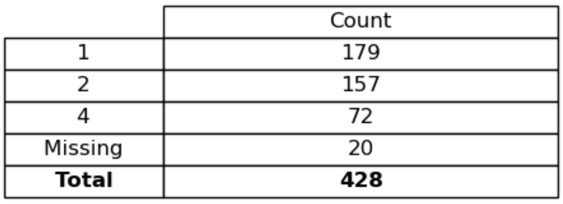


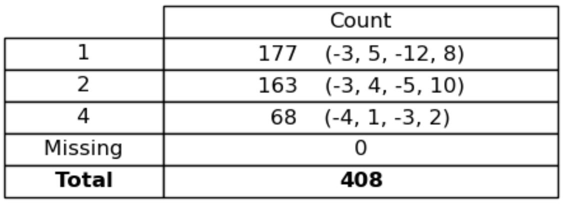
Figure 4: The k-means clusterings performed with $k = 3$, shown on the contingency table in Fig(3b), plotted on the first two principal components of the dataset shown in Fig(2).

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, which Fig(3) also provides subtle evidence in favour of this. 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



	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 remaining. 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.

opposed to the three clusters that the labelled dataset indicates.

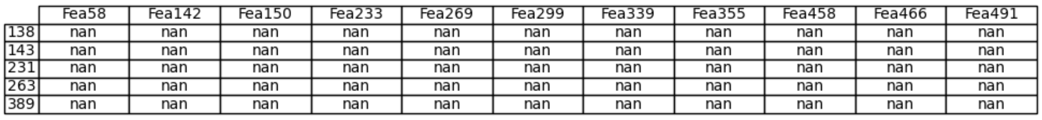
Performing k-means before PCA has the advantage of being able to visualise the cluster separation in the original feature space. However, this might not map well onto the PCA space, as the clusters may be more separable, or separate differently, in the original feature space compared to the 2-component 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 the raw `B_NoiseAdded.csv` dataset. 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.

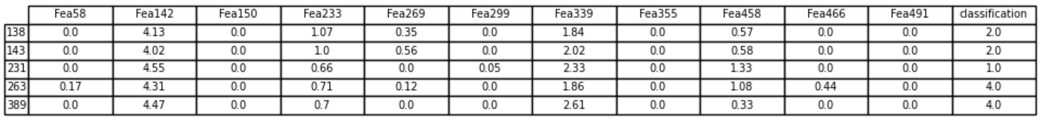
Several methods exist for handling missing labels. One method, model based imputation (used here), involves training a model on labelled data to predict missing labels. Alternatively, data with missing labels can be dropped, especially if the sample size is large. Whilst model based imputation utilises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

Missing at random (MAR) means a label's absence is unrelated to its value, whereas



	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 same samples, after imputing the missing values with PCA and KNN.

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

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 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 distinctly for each sample by 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 when the dimensionality is high w.r.t. the number of samples [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' [4], improving accuracy and aiding in identifying more meaningful neighbours. KNN imputation is preferable for clustered datasets where distance-based methods are effective and it is expected that nearest neighbours share similar properties.

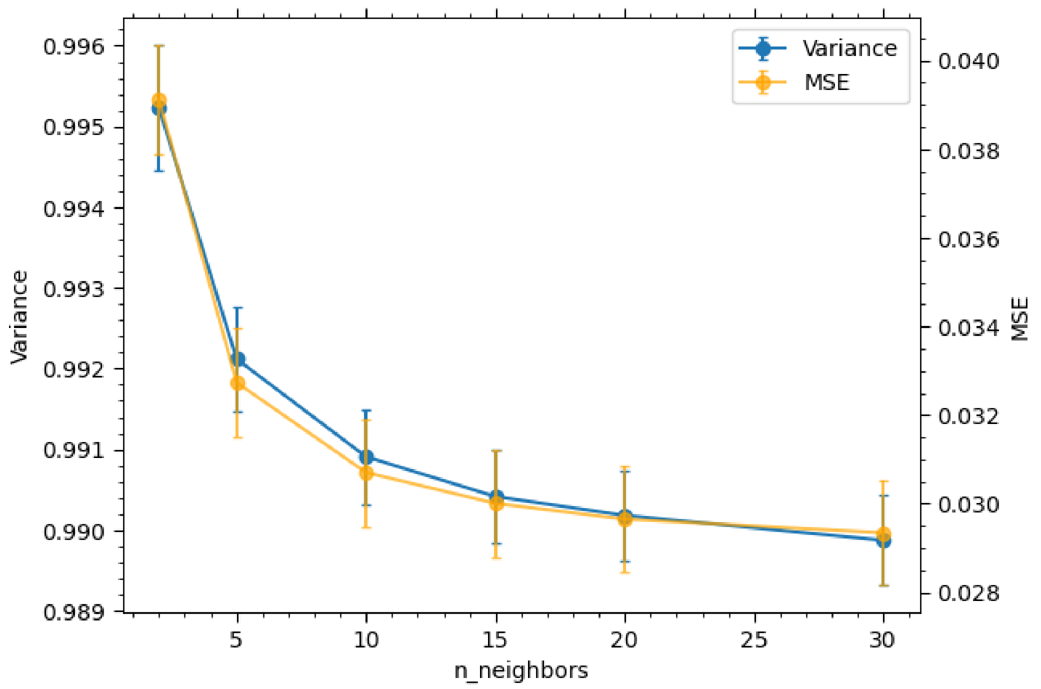
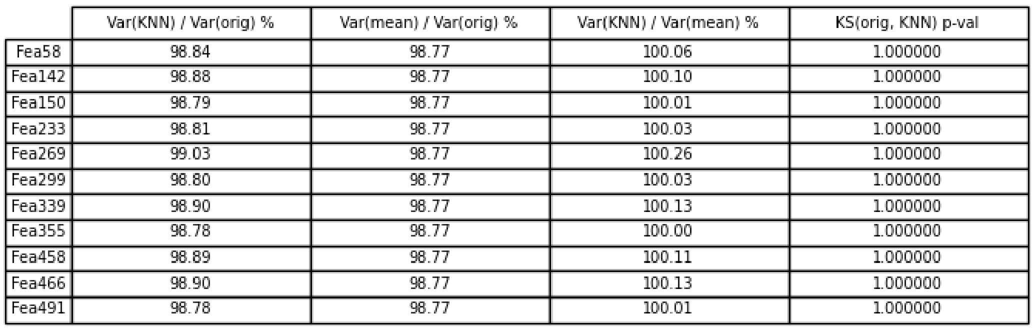


Figure 7: Variance and MSE of KNN imputed data, for different values of `n_neighbors`. The variance is shown as a percentage of the original dataset, and the MSE is the mean squared error of predicted values against the true values.



	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.

Fig.(6b) displays the data after missing values were imputed with PCA and KNN. Columns 1 and 4 in Fig.(8) indicate that this method largely preserved the original feature distributions, and column 3 indicates that this method preserved more of the original feature variance when compared to a static mean imputation.

1.3.3 Question 3d and 3e

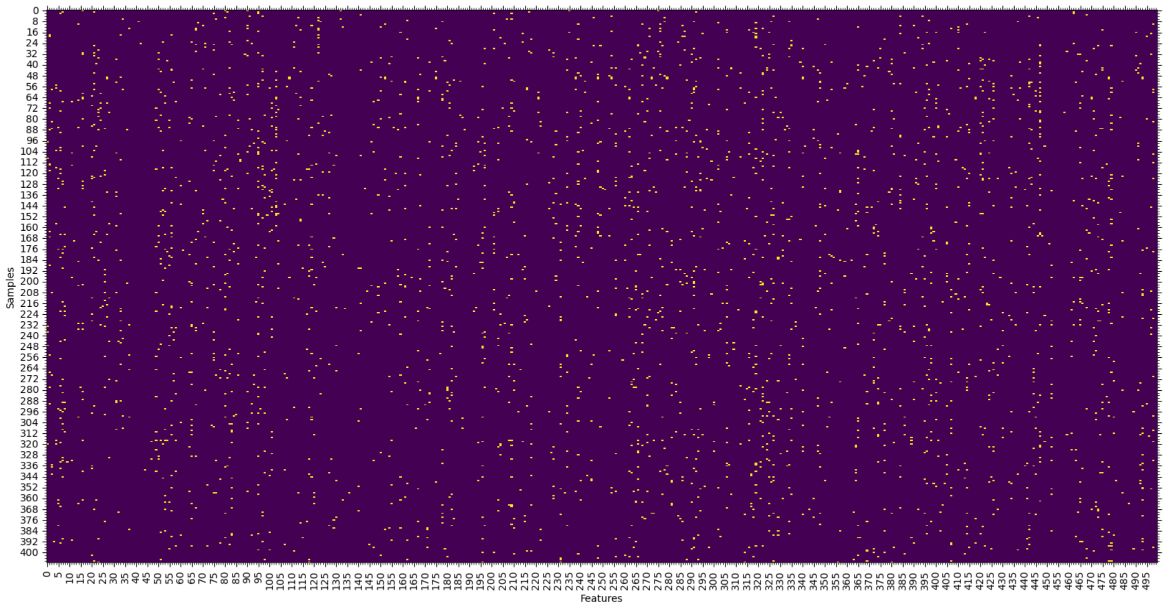


Figure 9: A heatmap of the outliers in the `C_MissingFeatures.csv` dataset. The orange marks indicate an outlier value, 2904 (1.42% of the values) outlier values were identified.

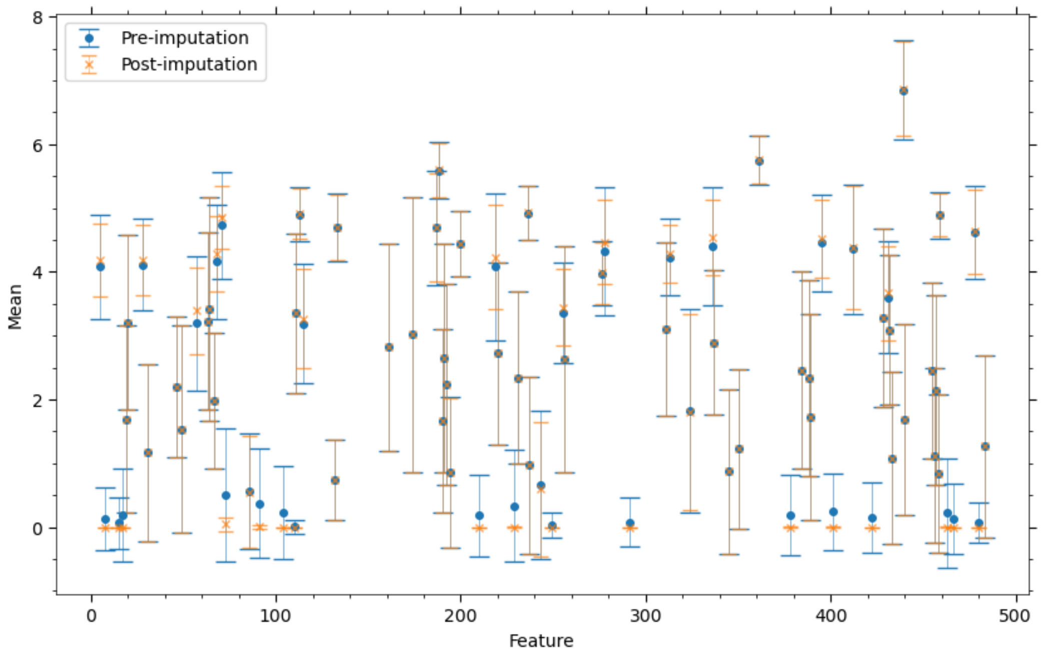


Figure 10: The mean and standard deviation of the 81 most discriminative features in the original `C_MissingFeatures.csv` dataset, before and after outlier imputation.

Outliers were identified by standardising the data feature-wise, and identifying values over 3σ from the mean. Fig.(9) indicates 2904 (1.42%) uniformly distributed outliers across the dataset.

These outliers were imputed using PCA and KNN, as in Question 3c, with the 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 only after 0.27% of the values 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. These 81 features were identified in the 2-component PCA space from the magnitude of the feature loadings before 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, briefly discussed in Q1a (Section (1.1.1)).

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. Each iteration splits a rectangle into two, based on a feature and a threshold. The final tree has N_n internal nodes, and $N_n + 1$ terminal nodes which represent the final classification: the modal class in that rectangle. Splits are assessed using criteria like the Gini index, choosing splits and thresholds that most reduce it. The Gini index [5], is:

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

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 exhibit high variance. Ensemble methods like bagging and random forests reduce this variance. Bagging trains multiple trees on bootstrapped training data, with classifications decided by majority vote. Random forests further lower variance by randomly selecting features for each internal node split, creating less correlated trees.

Two key hyperparameters in random forests are `max_depth` and `max_features`: the maximum internal nodes per tree and the number of features considered for splitting, respectively. Typically, `max_features` is set heuristically to $\sqrt{N}$, with N being the feature count.

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

The dataset underwent preprocessing with the outlier removal method from Q3 (Section 1.3), followed by standardisation. It had no duplicates or missing values. Due to imbalanced classes, stratified sampling was employed for train-test splitting.

The dataset was then classified using `RandomForestClassifier` and Fig.(11) shows a summary of the model performance. This gave a test set classification error of 10.0%.

The `RandomForestClassifier` was then optimised based on the out-of-bag (OOB) error rate. Results in Fig. (12) indicate that post 200 trees, the OOB error rate ceases to decrease significantly. Fig. (13) summarises model performance with 200 trees, showing the test set classification error improved to 8.6% and improvements in average precision, recall, and F1-scores.

	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: The confusion matrix and classification report averaged over 5-fold cross-validation for `ADS_baselineDataset.csv` using a random forest classifier. The leading diagonal show a mean 10.0% test set error. Matrix cells in (a) represent mean percentage allocations of the 100-sample test set, derived from a 0.8/0.2 train-test split.

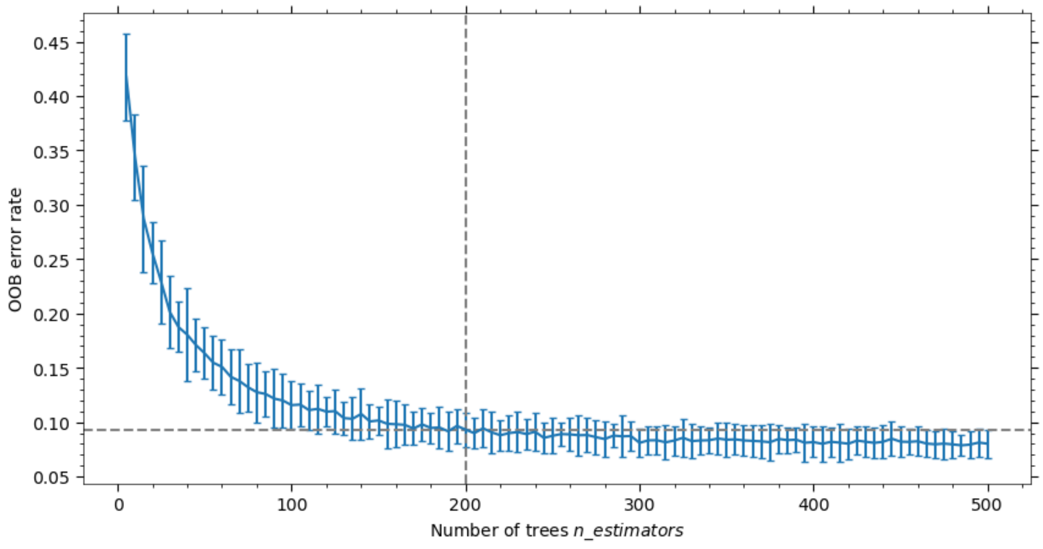


Figure 12: The out of bag error rate for a `RandomForestClassifier` on the pre-processed dataset `ADS_baselineDataset.csv`. The OOB error rate was computed 20 times per `n_estimators` to give error bars.

	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: Similar confusion matrix and classification reports as shown in Fig. (11), but with 200 trees. The mean test set classification error was 8.6%.

`RandomForestClassifier.feature_importances_` was used to calculate Gini importance (Fig. (14)). Gini importance measures the total normalised decrease in the Gini index due to internal splits on a feature. The top 322 features, representing 95% of cumulative Gini importance, were selected for re-classification (see Fig. (15)). Comparing Fig. (13) and Fig. (15), results were marginally better with the reduced feature set across all metrics

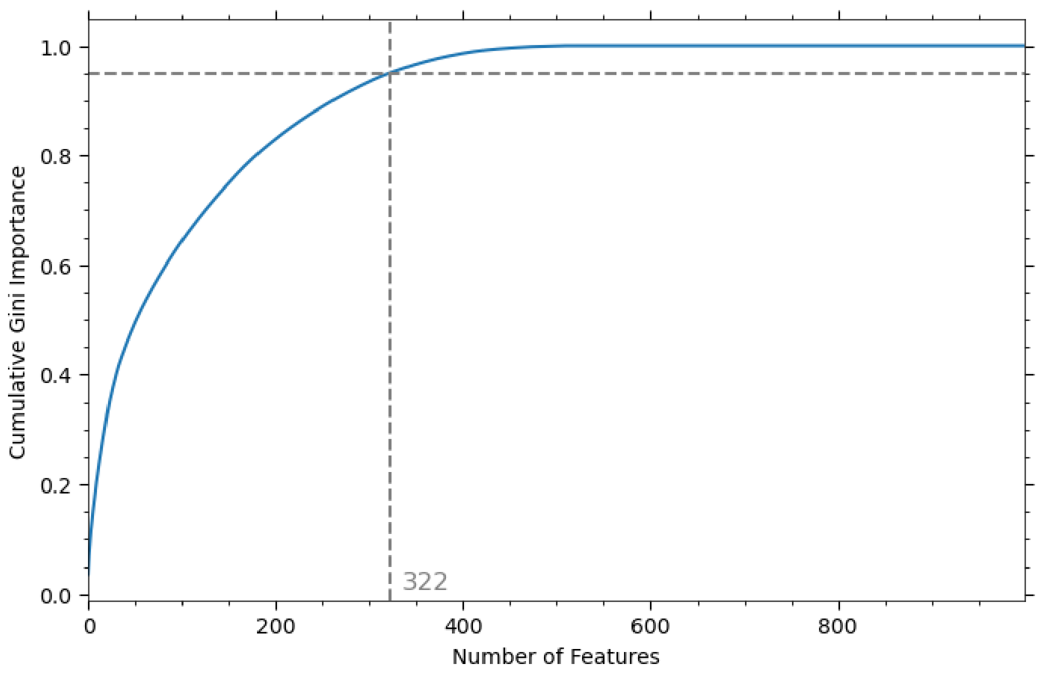
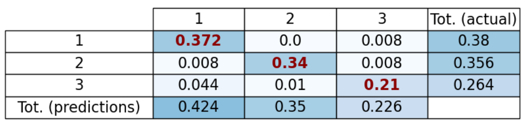
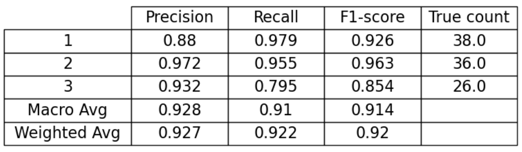


Figure 14: The ordered (highest first), cumulative Gini importance of the features in `ADS_baselineDataset.csv`. The horizontal grey line is the 95% threshold, which contains the top 322 features.



	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: Similar confusion matrix and classification reports as 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%.

2.1.3 Question 4f

The procedures outlined the previous section (Sec.(2.1.2)) were replicated using a multinomial logistic regression classifier, `LogisticRegression`. Fig.(16) and Fig.(17) illustrate the classification results using all features and the top 382 features, respectively. The latter demonstrates notably improved performance in test set classification error, precision, recall, and F1-scores. Feature importance was gauged using a novel metric, the normalised mean squared logit importance (NMSLI), calculated by averaging the squared coefficients for each feature across all 3 classes (`LogisticRegression.coef_`) and normalising them. This metric reflects the coefficient's magnitude and consistency across all classes, and was then treated like the Gini importance and the top 382 features were identified by calculating the features that contributed to 95% of the cumulative NMSLI (Fig.(18)). A comparison of Fig.(15) and Fig.(17) shows similar performance across all metrics for both reduced feature-

	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. Matrix cells in (a) represent mean percentage allocations of the 100-sample test set, derived from a 0.8/0.2 train-test split.

	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: Similar confusion matrix and classification reports as shown in Fig. (16) but with only the top 382 features. The mean test set classification error was 7.6%.

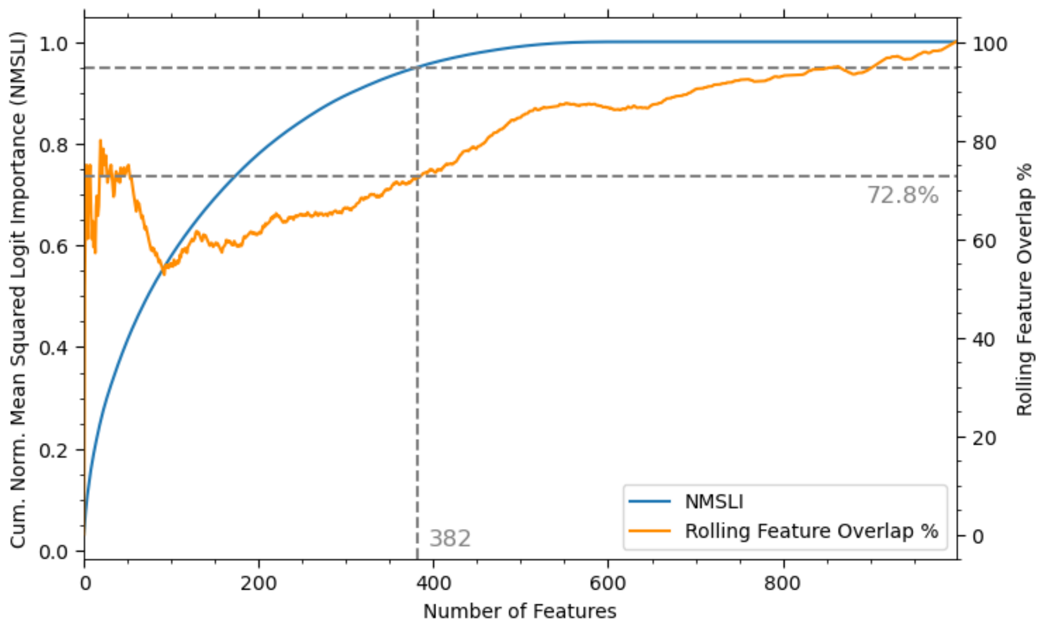


Figure 18: The ordered (highest first), cumulative NMSLI of the features in the `LogisticRegression` model. The top horizontal grey line is the 95% threshold, which contains the top 382 features. 72.8% of these 382 features were also in the top 382 features for the `RandomForestClassifier` indicated by the Gini importance (Fig. (14)) this is what the rolling feature overlap indicates.

set `RandomForestClassifier` and `LogisticRegression` models.

2.2 Q5 - Baseline Dataset

2.2.1 Question 5a

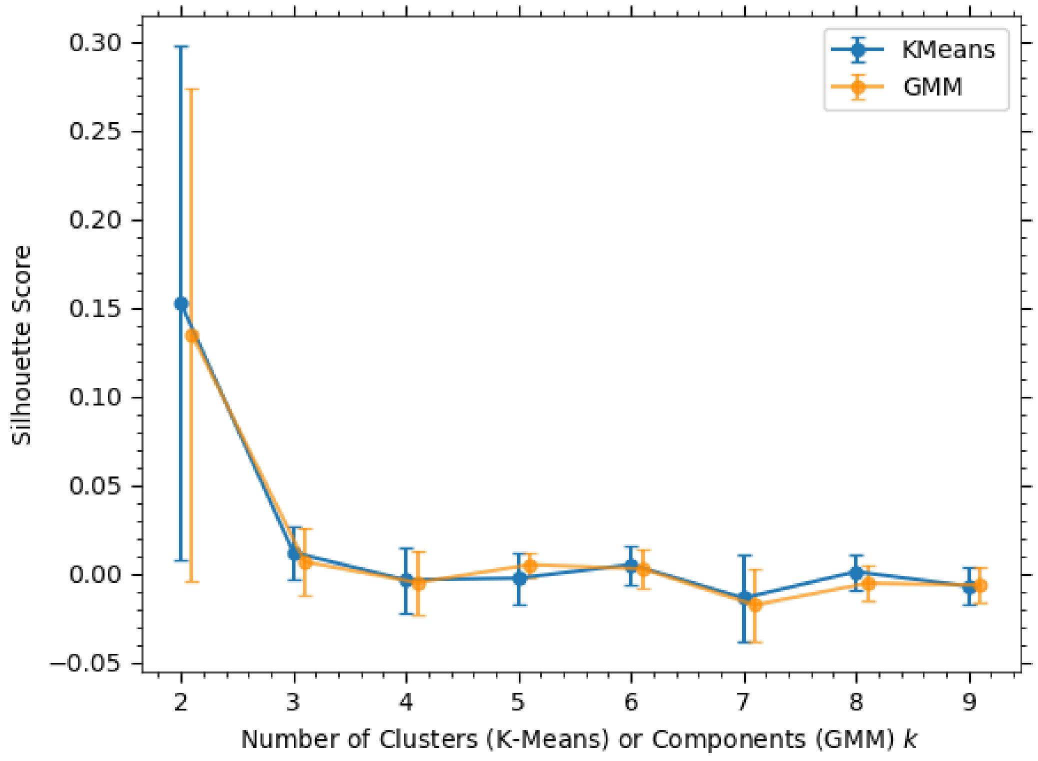


Figure 19: The silhouette scores for the `KMeans` and `GaussianMixture` models on the pre-processed `ADS_baselineDataset.csv` dataset. 5 repetitions were performed to give a mean and standard deviation for each k value.

The dataset `ADS_baselineDataset.csv` underwent identical pre-processing as for Q4, followed by the application of K-Means and Gaussian Mixture Models. `KMeans`, employing Lloyd's algorithm, produces k centroids, assigning each sample to the closest centroid, working under the assumption of a spherical data distribution. Conversely, `GaussianMixture` uses the expectation-maximisation algorithm to generate k Gaussian distributions, assigning samples based on highest probability. This allows for greater flexibility due to the Gaussian distributions' ability to model spherical and non-spherical data.

Fig. (19) displays the silhouette scores for both models, suggesting $k = 2$ as the optimal cluster number. However, significant errors at $k = 2$ highlight instability in locating a consistent solution for both models, as such, Fig. (20) examines the impact of increased initialisations on the cost function for both models. Both algorithms are very dependent on the random initialisation of the centroids/distributions and the disappearance of the error bars on both models at $n\_init > 10$ indicated that the algorithms required at least this many random initialisations to find the global minima. Therefore, $n\_init = 50$ was used hereon.

Fig. (21) presents a contingency table comparing cluster assignments of K-Means and Gaussian Mixture Models with these parameters, yielding an 87.2% agreement.

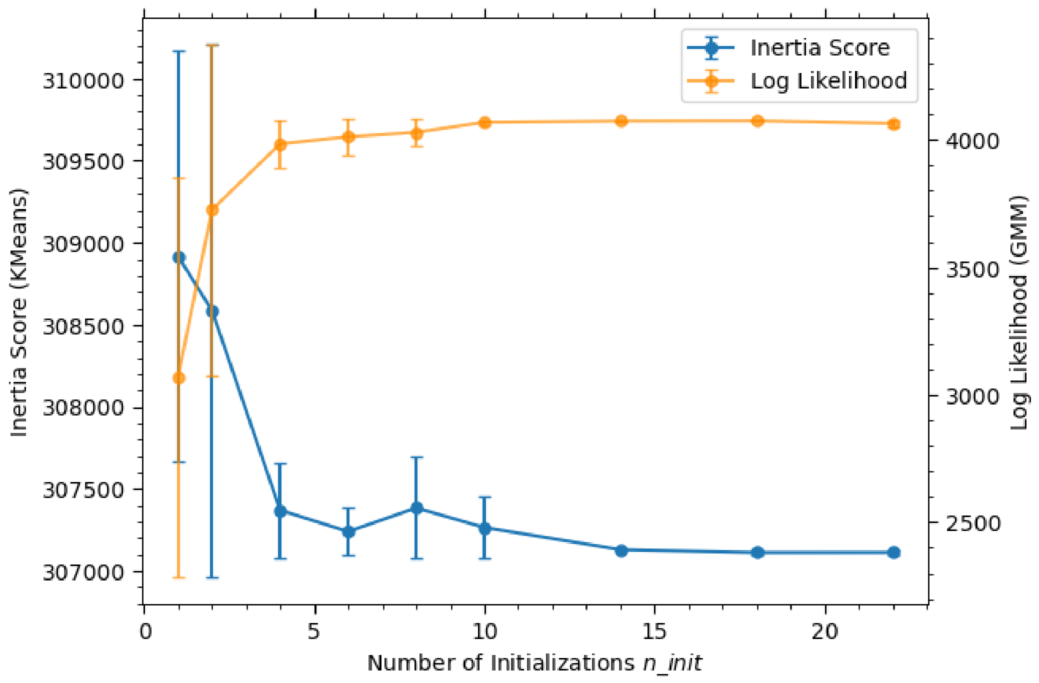
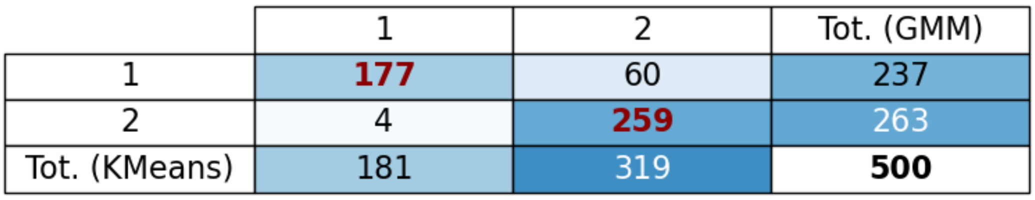


Figure 20: The cost functions for the `KMeans` and `GaussianMixture` models as `n_init` is increased, 5 repetitions were performed to give a mean and standard deviation for each `n_init` value.



	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 `KMeans` and `GaussianMixture` 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.

2.2.2 Question 5b

A `LogisticRegression` classifier was applied to the classifications in Fig. (21) to assess feature importance using the NMSLI metric, detailed in Section (2.1.3). This is depicted in Fig. (22). Subsequently, the top 295 features for `KMeans` and 298 for `GaussianMixture` were employed to retrain both models. The resultant contingency table, shown in Fig. (23), indicates a significant improvement with 96.6% agreement, surpassing the initial 87.2% agreement observed in Fig. (21).

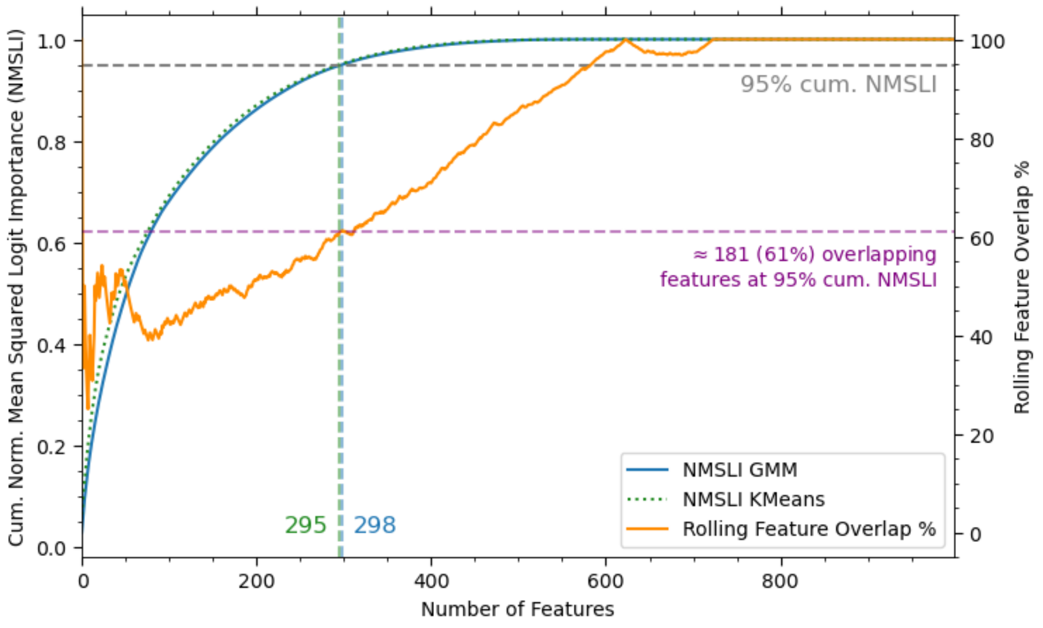
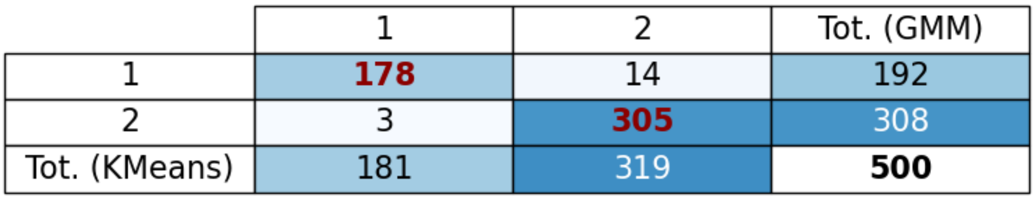


Figure 22: The feature importance for the `KMeans` and `GaussianMixture` models using a `LogisticRegression` classifier and the NMSLI metric on the classified data shown in Fig. (21). The 95% NMSLI threshold selected 295 and 298 important features for `KMeans` and `GaussianMixture` respectively, and 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 `KMeans` and `GaussianMixture` models after feature reduction as shown in Fig. (22). The leading diagonal shows a 96.6% agreement between the two models.

2.2.3 Question 5c

Fig. (24) presents the PCA visualisations of clusters identified by the k-means and Gaussian mixture models. The middle column reveals a strong positive correlation along $y = -x$ for the most discriminative feature, consistent across both models. The right column shows a slightly weaker positive correlation along the same line for the second most discriminative feature, which differed between the models.

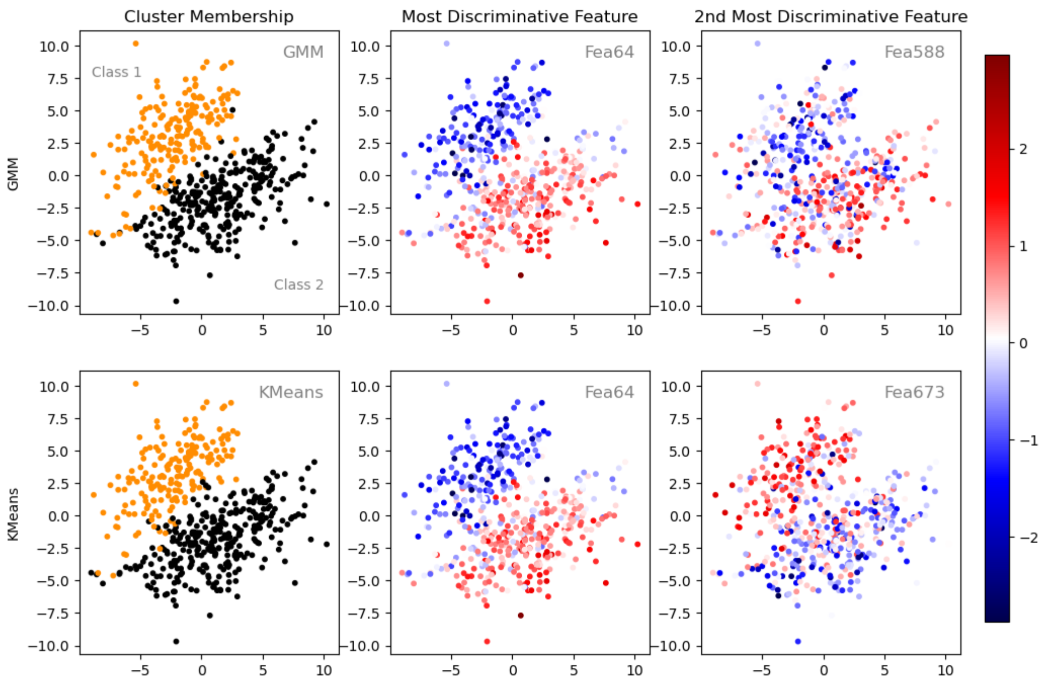


Figure 24: PCA visualisations of the clusters found by the K-Means and Gaussian Mixture Models as shown in Fig. (23). The top row is for the `GaussianMixture` model and the bottom row is for the `KMeans` model. The left column shows the cluster membership, the middle and right columns show the samples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

A Q2: Duplicate Observations in `B_NoiseAdded.csv`

The 20 duplicated pairs in `B_NoiseAdded.csv`, the numbers are the sample numbers, which is 1 higher than the row number in the dataset: [[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]]

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