Q1 - Visualization and analysis of the Palmer dataset

The Palmer penguin dataset consists of 344 records of the physical attributes of three species of penguin living on three islands in Antarctica (Table 1) [1]. In this report, consideration is given to data cleaning and preparation, the dataset is explored through visualization and analysis is carried out to compare the accuracy performances of a small number of AI approaches.

Feature	Type	Values in the dataset	Importance
island	categorial	Torgersen, Biscoe, Dream	0.13
bill length	numerical	32.1mm - 59.6mm	0.16
bill depth	numerical	13.1mm - 21.5mm	0.02
flipper length	numerical	172mm - 231mm	0.65
body mass	numerical	2700g - 6300g	0.01
sex	categorial	Male, Female	0.04
species	categorial	Adelie, Chinstrap, Gentoo	class

Table 1: Attributes of the Palmer penguin dataset. Importance is calculated using random forest.

Data cleaning - missing values, encoding, standardization and imbalance

The two records missing the sex amd all numerical features were removed as imputation is unlikely to be reliable. The remaining nine records are missing only the sex attribute. Figure 1 shows the physical attributes of the male and female of each species differ statistically and so it is reasonable to consider imputing sex for those records. Following standardization, a Shapiro-Wilk test confirmed each numerical attribute has a normal distribution [2] and separate Z-tests were applied to assess the hypotheses that the missing sex value is male or female [3]. Two of the records could be imputed as male and three as female and these were retained. with the remaining four records being removed. The cleaned dataset has 338 records, 147 Adelie (74 male, 73 female), 68 Chinstrap (34 male, 34 female) and 123 Gentoo (62 male, 61 female).

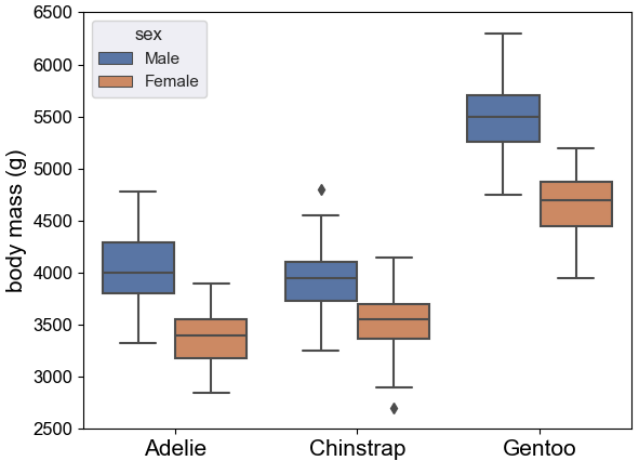


Figure 1: All numerical features show a significant statistical difference between male and female, as in the body mass above. Shown are median values, upper and lower quartiles, and outliers.

The categorical features in the dataset were encoded to numerical values. 'One-shot' encoding of categorical features was not found to improve performance. A number of AI methods are known to be biased in favour of numerical features with smaller standard deviations [4], but this can be reduced by standardization of features to zero mean and unity standard deviation. Standardization statistics are calculated only from the training set, but are also applied to the test set. If a dataset is imbalanced, AI predictions may be biased towards classes more frequently found in the training data. In the Palmer penguin dataset, the number of Chinstrap records is around half of that of both Adelie and Gentoo, but, as all the methods adopted in the current work are known to be little affected by imbalanced data [5], no modifications were made.

Visualization of the dataset

Figure 2 shows the species distribution for the islands. Chinstrap and Gentoo penguins are found only on one island, making island a potential confounding factor whose individual environmental factors may influence physical characteristics. A Shapiro-Wilk test confirmed the normal distribution of the numerical features of the Adelie penguins (found on all islands) and an ANOVA test

confirmed the features are not significantly influenced by the island inhabited. Consequently, the island is not a confounding factor in the dataset.

The feature importance scores in Table 1 represent relative contributions in predicting the species and were calculated using a random forest approach. Results reported later show that performance improvements can be achieved by concentrating classification on the more important features.

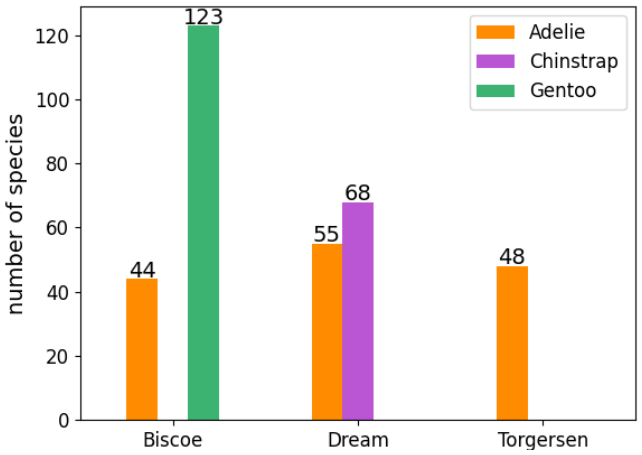


Figure 2: Adelie samples are from all three islands, but Gentoo and Chinstrap from only one

The pairwise scatterplots for the numerical features are shown in Figure 3. Bill depth, in combination with either flipper length or body mass, yields a separable cluster of Gentoo penguins (shown in green) allowing them to be identified. No pairwise combination completely separates Adelie (orange) from Chinstrap (purple) clusters, but the best candidate feature for doing so is in the distributions involving bill length.

Figure 1 above shows there is a difference in the body masses of the male and female samples for each of the three species. Differences between the sexes for the other three numerical physical characteristics in the dataset were also apparent. Since narrower distributions are apparent if the sex of the species is considered rather than just the species itself, including sex is likely to provide a finer grained distinction for species classification and this knowledge can be used to improve performance, as discussed in the analysis section below.

Methodology

All code is in Python 3.11 [6] using 'Scikit-Learn' libraries [7] under Ubuntu Linux [8]. The code is available in a Gitub repository [9]. Predicting the penguin species from the given features is a classification problem. Results are obtained from a baseline method, two convention classification approaches, namely k-Nearest Neighbour ($k$nn) [10] and random forest [11], unsupervised k-means (following cluster labelling) [12] and a novel combined visualization and analysis (CVA) approach that uses practical visualizations and Support Vector Machine (SVM) classification.

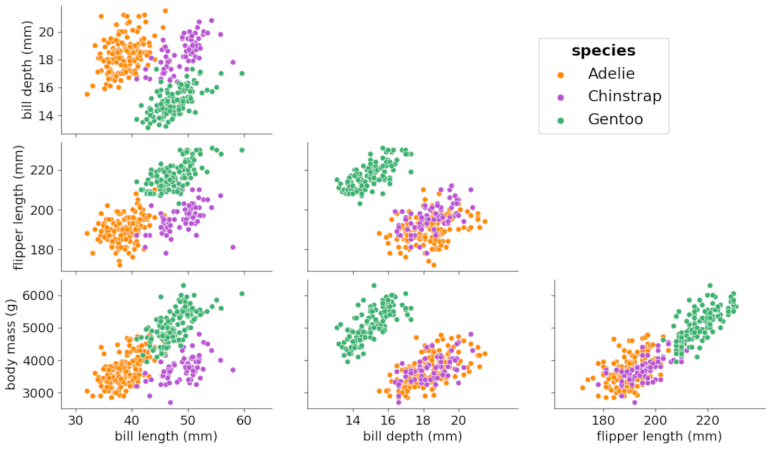


Figure 3: Pairwise distributions of numerical features. Gentoo can be distinguished, but Adelie and Chinstrap may not be completely separable from one another

To reduce the potential for overfitting, the classification methods (all but k-means) were trained using 'holdout validation', where 80% of the dataset was used in a five-fold cross-validation configuration [13]. The remaining 20% was kept for a test set. For all methods, the Scikit-Learn function GridSearchCV was employed to tune metaparameters [7]. Table 2 shows the values selected for the metaparameter grid. Those giving the best performance were selected to generate accuracy results (the percentage of correctly predicted species) from the test set. Calculation of the metrics

'precision' and 'recall' were also considered, but these are only relevant if false positives or false negatives (respectively) are to be avoided.

Results and analysis

Scikit-Learn provides pseudo-random procedures for selecting validation and test set values and 100 of these were used both when selecting metaparameters and when deriving accuracy results.

The results in Table 3 include a baseline that is used to demonstrate performance improvements achieved by the AI methods being considered. In classification, the baseline method is often simply to select the most frequent class in the observations and, in this work, this is the Adelie penguins, giving an accuracy of 43.49% (147/338).

Method	Metaparameters	Values considered
$k$nn	nearest neighbours k	***1***, 2, 3, 4, 5, 6, 8, 10
	prediction weight function	***uniform***, distance
	neighbours distance metric	**Manhattan**, Euclidean
random forest	trees in the forest	5, ***10***, 15, 20, 25
	maximum depth of trees	***no maximum***, 10, 20
	min samples to split node	***2***, 5, 10
	min samples at leaf node	***1***, 2, 4
	quality of split function	***gini***, entropy
k-means	number of clusters k	2, ***3***, 4, 5, 6, 7, 8, 9, 10
	centroid initialization	***k-means++***, random
	runs for centroid seeds	2, ***5***, 10, 20
	max number of iterations	5, ***10***, 20, 50
CVA	regularization parameter	0.1, 1, ***10***, 100
	kernel coefficient	***1***, 0.1, 0.01, 0.001
	kernel type	rbf, ***linear***, polynomial

Table 2: Metaparameters values shown in italics most consistently produced training results of best accuracy during validation and were selected for generating results

Method	Accuracy
baseline, most numerous species	43.49%
kNN, all features	99.24%
kNN, no island	99.46%
random forest, all features	98.57%
random forest, three features	98.57%
k-means, numerical features	97.06%
k-means, sex clusters	98.23%
CVA, three main features	98.56%
CVA, as above but with sex	98.78%

Table 3: Mean classification accuracy from 100 test sets each generated by a pseudo random approach and using the parameters identified in Table 2

Classification method 1 - *k*nn The performance of $k$nn was found to be improved by omitting features from training. An exhaustive search involving omitting all combinations of features in turn determined that the best accuracy was obtained when island was omitted and this occurred when k=3. It appears that island was not providing any additional information and the higher value of k implies better generalization may have been achieved.

Classification method 2 - Random forest Including all of the features in the analysis gave an accuracy marginally better than achieved using $k$nn. I contrast to $k$nn, no performance improvement was found using fewer features, indicating that considerably less implementation effort is needed to achieve good performance using random forest. A marginal improvement in performance was apparent when island, flipper length or body mass were not included in training.

Unsupervised method - *k*-means Although an unsupervised clustering method, k-means can be used for classification by matching clusters to classes. The k-means method is normally applied only to numerical features so only they were included in this work. The number of clusters (k) can be selected using elbow and silhouette methods, as shown in Figure 4. Empirically, accuracy improved significantly when $k \geq 4$ as clusters were not reliably formed for all three species for smaller values of k, Figure 5 illustrates the mapping of classes to clusters for two feature dimensions. No improvement in accuracy was obtained by reducing the number

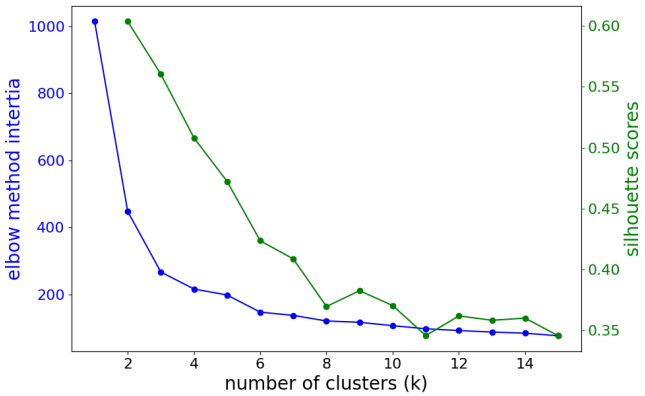


Figure 4: The k-means elbow is the change in slope of 'inertia' (k=3) and the silhouette is the 'score' closest to 1 (k=2)

of features, but, in an additional experiment, a set of k-means clusters was created for each sex and this led to a small improvement in accuracy.

A novel combined visualization and analysis (CVA) approach The CVA approach involves visualizing pairwise plots of features to identify a sequence of two-dimensional SVM classifiers. CVA requires manual effort to understand the nature of the dataset, in contrast with 'black box' classification approaches that can be applied with limited knowledge of the method and little insight into the nature of the data. The main drawback of the CVA approach is that it may not always be feasible to extract the necessary visualizations insights particularly for large dimensional datasets.

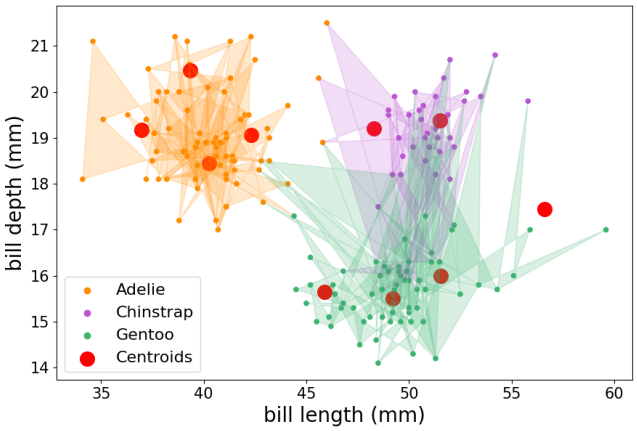
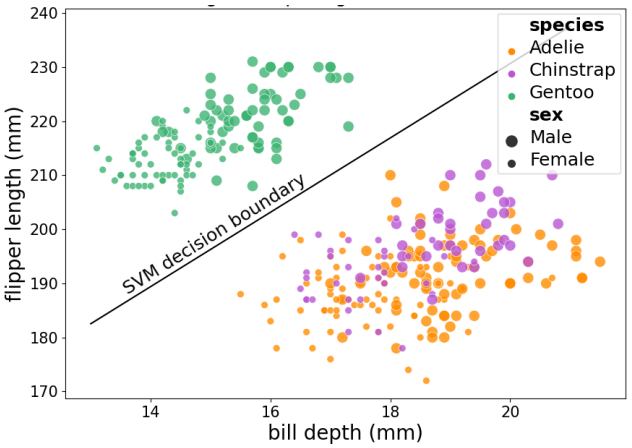
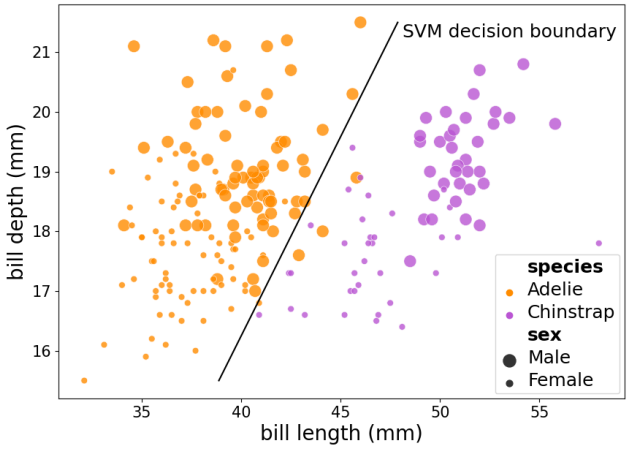


Figure 5: k-means clusters mapped to species using majority voting. Class assignments are shown by polygon colour (k=10, 50 samples coloured).

An application of CVA to the Penguin dataset is illustrated in Figure 6. Figure 6a shows the relationship between bill depth and flipper length and SVM is used to find a suitable 'decision boundary' that separates Gentoo from the other two species. Figure 6b then shows a second SVM line that best separates Adelie and Chinstrap using bill length and bill depth. CVA was able to produce results of accuracy almost as good as conventional approaches and a small improvement was apparent when separate SVM models were developed for each penguin sex.



(a) Gentoo can be distingushed from other species



(b) Adelie and Chinstrap can be partially separated

Figure 6: Two-stage CVA approach with boundaries fitted using SVM to training data of feature pairs

Conclusions

With careful data preparation, optimization of metaparameters and robust application of training and testing methods, the $k$nn and random forest classification methods produced high-quality results. As expected, the k-means accuracy results were comparitively worse as it does not take advantage of target data information known to the supervised approaches.

The novel CVA approach was able to produce accuracy results similar to those of other classification methods. Although needing to be tailored to each problem and not well-suited to high-dimensionality data, its internal operations are transparent and this is in contrast with general-purpose classification methods.

A classifier that is able to achieve 100% accuracy for the given data is possible, but is likely exhibit poor generalization.

References

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