Can machine learning be used to identify species of Sorbus

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Pl. 113. Sorbier des Oiseleurs. Sorbus aucuparia L.

0. Abstract.

There are many reports in the literature of machine learning as a method of identifying plants using visual images of leaf or flowers, for example,(Gwo and Wei 2013,Valliannal and Geethalakshmi (2012)). However, the use of morphological features is less well documented. Three algorithms were used to separate seven species of *Sorbus* within the subgenus *Soraria* based on morphological measurements of fruit and leaves. Two unsupervised clustering techniques, namely K-means and hierarchical clustering and one supervised decision tree. Box plots showed considerable overlap of characteristics between the species, but that some species were differentiated in one or two characteristics, suggesting clustering techniques would be less successful than decision tree methods. This was seen in the results with K-means modelling being unstable and unable to repeatedly produce accurate results. Hierarchical clustering using the canberra distance metric gave an accuracy of 0.42 while precision ranged from 0 to 0.81 and sensitivity from 0 to 0.87 using non-standardized data. A decision tree was the most successful method giving an accuracy of 0.68 with precision ranging from 0.4 to 1 and sensitivity from 0.17 to 0.85.

1. Introduction - The genus *Sorbus*.

Sorbus is a member of the Rosaceae family, perhaps the best known species being *Sorbus aucuparia*, the Rowan or Mountain Ash. However, there are over 50 species of *Sorbus* in the UK, (NBN 2018), 38 of these are vulnerable or critically endangered and most are endemic or native (Rich et al. 2010). There are four diploid species, but, as with many Rosaceae, *Sorbus* produce new apomictic polyploid species, (Robertson et al. 2016). These can also produce viable pollen and can therefore back-cross with other diploid or polyploid species,(Ludwig 2013). This results in a large number of genetically unique, stable, clonal communities, which can look very similar to each other. This presents a problem with recording and many *Sorbus* require expert knowledge to correctly identify to species level because much of the identification depends on comparative knowledge, (Rich and Jermy 1998). This tends to dissuade recorders, or encourages records at aggregate level. This is a problem for such an important genus with many endangered plants that could benefit from identification.

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Sorbus are grouped into six subgenera, each of which are reasonably easy to identify by recorders with some knowledge. More difficulty arises when identifying plants within these subgenera, and this is where this work has concentrated. In this modelling only the subgenus *Soraria* has been trialed. This subgenus consists of eight species all similar in appearance to *Sorbus intermedia*, although only seven species are considered based on the availability of data. These plants are distinguished from other subgenera by having leaves with rounded lobes which are tomentose beneath and the fruits having fewer lenticles. Perhaps the most noticeable difference between plants within the subgenus are the larger fruits on *S. intermedia*, the smaller leaves of *S. minima* and the small fruits of *S. mougeotii*.

2. Data and data preparation

The data was provided by Dr T Rich, the Botanical Society of Britain and Ireland expert on *Sorbus* and consists of leaf and fruit measurements. For the leaves, the length, width, widest point on the leaf, base angle, number of veins, depth of the lobes, and vein angle have been recorded. For the fruit, the length and the width are used. Due to the variability in leaf size across one plant, the measurements were all carried out in a specific manner described by Rich et al, (Rich et al. 2010). Essentially, repeated measurements of the central leaves on sterile spurs on the sunlight side of the tree are recorded and averaged over at least ten leaves.

The nature of collection means that the data was sparse. Not every plant in each species had a complete set of measurements or the same number of records as other species. For example, *S. intermedia* had 126 observations but *S leyana* only had 39. This is due to the relative occurrence of the two species. *S. intermedia* is a common plant found throughout the UK in easily accessible places, whilst *S. leyana* is only found in two sites in South Wales, sometimes on the sides of cliffs. In addition, measurements cannot all be collected at the same time. Leaves must be measured when mature, around flowering time, and therefore cannot be measured in conjunction with fruit. Separate trips to re-measure fruit on the same trees may not be possible. For *S. intermedia*, for example, of 122 records, 72 are purely for fruit measurements and the remaining 50 purely for leaf measurements, and these occur on different plants If imputation was carried out, 59% of the leaf

measurements would be imputed, which would be detrimental to the accuracy of the model, (Peters 2005). Initial data exploration did find this reduced the accuracy of K-means.

Therefore, the sparsity was handled in two ways. Firstly, by reallocating measurements. For example, the 50 leaf measurements for *S. intermedia* were assigned to 50 fruit measurements and the excess 22 were not used. Secondly, for some species, where there were only a few additional rows of incomplete data, median imputation was carried out.

Although it seems dubious to assign records from one plant to another, in this analysis this was felt to be acceptable for two reasons. Firstly, this project focuses on modelling techniques and an initial exploration of machine learning methods; it is not intended as a complete and accurate method for species identification at this stage. Secondly, the clonal nature of these plants implies that we would expect a great deal of similarity within a species. However, if these plants are phenotypically very plastic, this assumption may be invalid. The range of leaf sizes within each plant was not available, so a comparison of the variation within each plant and between all the plants of each species would be useful here.

This data handling procedure also has the benefit of producing a data-set with no missing values, and some of the machine learning algorithms used here had no method for dealing with these, hence they must be removed before modelling. Clustering algorithms, because they rely on distance metrics, are usually sensitive to scale in the data,(Ismail 2013), therefore the data was also standardized and each clustering model carried out on both standardized and non-standardized data. Since standardization should not effect a decision tree, (Nisbet, Miner, and Yale 2017), only the non-standardized data was modeled.

Because each species had a different number of records a random stratified sampling system was carried out to create train and test sets used in the supervised leaning algorithm in which each species was split into 70/30 train/test sets.

3. Modelling

3.1. Model performance metrics

In supervised learning, the correct and incorrect values assigned to each class are known, and these are used to evaluate the model by calculating accuracy, precision and sensitivity.

Accuracy is is the number of correct values divided by total number of items evaluated.

Precision is the true positive rate of a predicted class. The precision for a species tells you how accurately the algorithm is identifying a species, a low precision tells you that other species are incorrectly lumped with the correct species. A high precision tells you that most of the species are correctly identified and that the predicted class will be predominantly made up of the right species.

Sensitivity is the true positive rate of a species. A low number tells you the correct species have been put in other, incorrect, classes. A high sensitivity tells you that most of the species have been put in the right class, and that most of the actual species are in the correct predicted class.

Actually, despite using a mixture of unsupervised and supervised learning methods, we do know the identification of the species, so in fact we can also calculate accuracy, precision and sensitivity for the unsupervised models and hence compare all models using the same metric.

In addition, clustering algorithms can use various other metrics, such as the ratio of within cluster sum of squares to total sum of squares to evaluate the model. For well defined, compact clusters the ratio will be small. Since this metric was not available for all models, it is not used to compare different models. In addition, since the two clustering techniques performed so poorly, there was no reason to compare the two, and therefore these metrics are not shown here.

Confusion matrices, which summarize the the frequencies of the species allocated to different classes and clusters, were produced to examine two of the models, but they were unfeasible for the K-means algorithms since this was repeated ten times, as discussed below, and the large number of confusion matrices would obfuscate the results. Since they give the same information as accuracy, precision and sensitivity, they were used to discuss hierarchical clustering and the decision tree, but not to compare models or examine the results of K-means.

3.2 Modelling methods.

Three machine learning methods were used; K-means, hierarchical clustering and a decision tree. The first two being unsupervised clustering techniques and the third a supervised classification algorithm.

3.2.1.Decision tree.

Variables are used to make binary decisions as to whether data points are part of a group or not. Splits are made based on whether the information after the decision, i.e., the separation of the groups, is increased or decreased. The final classes would ideally contain only the items of a single species, this will rarely be the case due to noise within the data. The model here is represented by the logical processes followed to reach the final classes. The rpart package was used for the decision tree, (Therneau, Atkinson, and Ripley 2018). The rpart library also offers a decision tree plot which summarizes the binary choices used at each node.

3.2.2. K-means

K-means is an unsupervised clustering technique. Even though we do know the identity of the instances in the data, this is not used in the model. Instead, the data is grouped into clusters where the aim is to make the items within each cluster similar, whilst each cluster is as dissimilar as possible from other clusters. This is similar to a classification technique except the classes to which the items belong are not specified. In clustering, no information is needed about the objects and there is no right or wrong, so in that sense, our problem does not demand clustering. We know what species a sample belongs to and we do not want it allocated to another cluster. However, it is a useful technique to see if the model reflects the patterns we know the data contains. The K in K-means refers to the number of clusters to be used, which, because we know the data contains seven species we specified as such.

In K-means k centroids are randomly assigned to the data. The data points are then assigned to the closest centroid, resulting in k clusters. The centroid is then moved to the average location of

the data-points in its cluster. This process is repeated until the centroid position is stable, or the maximum number of iterations has occurred. If repeating the K-means function results in different clusters, which can be seen in differences in accuracy, it can be assumed that the algorithm is not efficient at separating clusters. Since the number of clusters is known, repeating the algorithm with k = 7 and examining the accuracy on each repeat will indicate the success of the model. Ten repeats of the model were carried out and the accuracy calculated on each run.

3.2.3. Hierarchical Clustering.

Bottom up hierarchical clustering assigns each data-point to a single cluster, the distance between the clusters is calculated and the closest two points are aggregated into a new cluster, so the clusters decrease by one. The process is repeated until all items are clustered into one. The clusters can be cut at k = 7 and the members examined. Hierarchical clustering was explored using different distance methods in order to ascertain the method giving the highest accuracy and this method was then used to calculate precision and sensitivity. The hclust function was used which is part of the stats package which is usually included in base R.

3.4 Computing languages

R was the main language used in this project within Rstudio, (RStudio Team 2016) although there is no reason, in terms of functionality, why python could not be used. A benefit of R was that it can easily be used in conjunction with R markdown, which is used by the data providers and who may want to modify the model. If the focus of the project had been machine learning itself, the caret package (Kuhn 2017) would have been more efficient than the methods written here; it provides hundreds of algorithms, training options, plotting and cross fold validation all wrapped up within its functions. The package would allow more thorough and robust models to be produced.

A python script was used to compile the markdown file, which has the benefit of allowing neater folders. For example, compiling within Rstudio will not always retrieve images from folders other than the working directory, and therefore the Code directory can become cluttered with non-code files. Using a python compilation script means the image files can be stored outside the Code

161 directory and moved in and out when compiling.

162 Bash was used to render the rmarkdown file because python would not easily handle the syntax of
163 the command. This was not a problem in bash and it was therefore easier to incorporate one line of
164 a bash call within the python script for this.

165 R markdown was used as it provides the same functionality as Latex, allowing the use of Latex
166 commands directly within the document, but with the added benefit of being a dynamic document
167 that is commonly used by other researchers in ecology, and in particular, the data providers.

168 4.Data exploration.

169 If the data is separated into clearly defined groups, we can be sure that a clustering algorithm will
170 work. Box plots are presented for the standardized, which is used for the clustering algorithms and
171 non-standardized data used in the decision tree. The plots show that certain features are clearly
172 differentiate in certain species. For instance, fruit width would separate *S. anglica*, and then fruit
173 length would subsequently separate *S. leyana*. This suggests that a decision tree algorithm could be
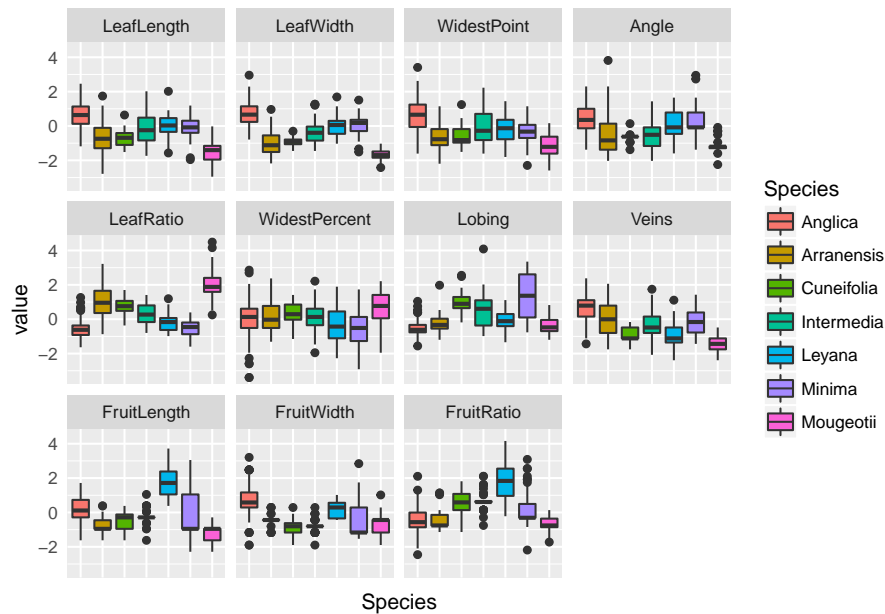174 successful.

Figure 1: Box plots for standardized data. There is alot of overlap between the species. FS leyana
stands out as having longer fruits and S anglica with its larger leaves. The leaf ratio separates S
mougeotti because of its very lanceolate leaf. But the other species overlap in most variables
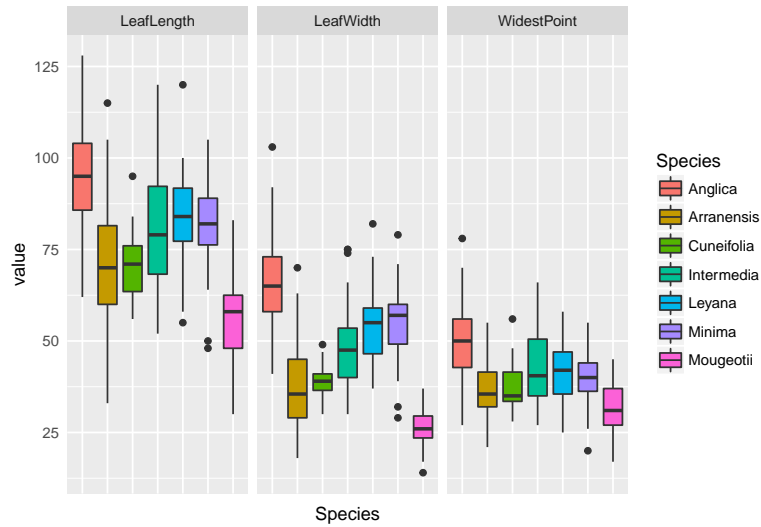
Figure 2: Box plots for non-standardized data: Leaf length and width,and position of widest point. Leaf width and leaf length separate S. mougeotti and S anglica with their very narrow and very wide leaves, the other variables show a lot of overlap
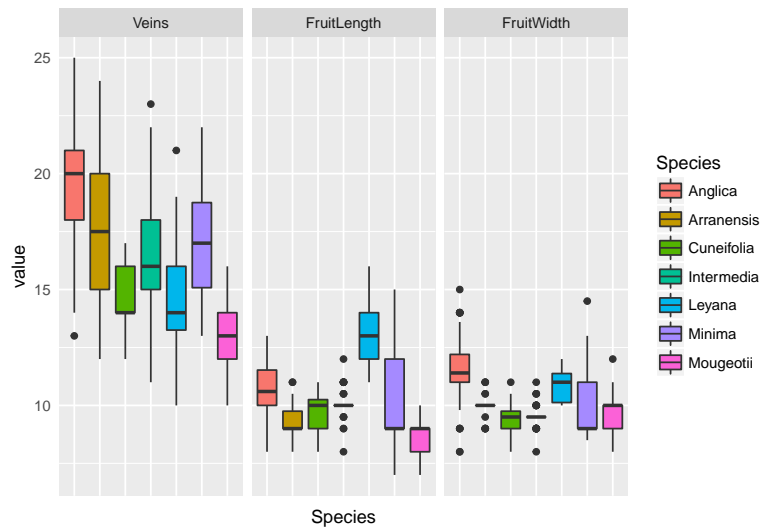
Figure 3: Box plots for non-standardized data: number of veins,fruit length and fruit width. Fruit length separates S leyana, which has very long fruits and S mougeotti, which has very short fruits. There is a lot of overlap between species in the number of veins
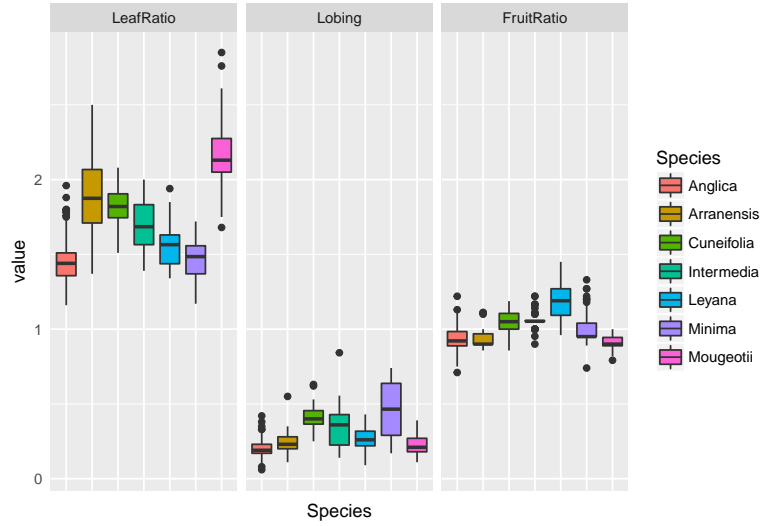
Figure 4: Box plots for non-standardized data: ratio of fruit length and width, ratio of leaf length and width and depth of lobes. S mougeotti stands out as having lanceolate leaves whereas those of S anglica are more ovate.

5. Results

Since the output of the machine learning algorithms is mainly in the form of tables, many of these have been placed in the appendices for clarity. A couple of exemplar tables only are used in the results section.

5.1 Kmeans

Table 1: Accuracy

	Run 1	Run 2	Run 3	Run 4	Run 5	Run 6	Run 7	Run 8	Run 9	Run 10
unstandardized	0.14	0.27	0.15	0.09	0.14	0.12	0.22	0.09	0.14	0.12
standardized	0.02	0.08	0.07	0.10	0.29	0.09	0.33	0.06	0.02	0.14

The accuracy shown in table 1 is different on each run implying that the algorithm is not successfully grouping the data into the same clusters.

Tables 8 to 11 in Appendix I show the sensitivity and precision for ten runs of the model. 100% sensitivity and precision could be achieved on some runs for some species, for example for *S. arranensis* using standardized data, but this was not seen in other species and in a subsequent run this would drop to 0.

In summary, K-means is not consistent across species, does not achieve high accuracy and is not repeatable.

5.2 Hierarchical Clustering

Table 2: Accuracy obtained in hierarchical clustering using different distance metrics for non standarized data

Distance Method	euclidean	maximum	manhattan	canberra	minkowski
Accuracy	0.3	0.18	0.29	0.42	0.3

Table 3: Confusion matrix for Canberra method using non-standardized data

	1	2	3	4	5	6	7
Anglica	108	41	11	0	0	0	0
Arranensis	7	14	0	0	22	0	7
Cuneifolia	0	1	0	8	10	0	0
Intermedia	13	2	2	22	8	1	0
Leyana	4	17	6	0	0	3	0
Minima	1	8	9	29	0	3	0
Mougeotii	0	0	0	0	12	0	11

Table 2 shows that the Canberra metric gives an accuracy of 0.42 for the non-standardized data. The Euclidean and Minkowski methods give slightly worse accuracy of 0.41 for the standardized data, shown in table 12 of Appendix II. As in K-means, the performance of the standardized and non-standardized data is contrary to expectations, with the standardized data not giving obviously better results.

The confusion matrix in table 3 shows that while 69% of *S. anglica* is allocated to the correct class, for *S. arranensis, S. leyana* and *S. minima* this number is 0% or nearly so. The confusion matrix for the standardized data shown in table 13 of Appendix II does not show markedly better results.

The sensitivity and precision calculated for standardized and non-standardized data are shown in tables 14 and 15. The results are again inconsistent, a high precision and sensitivity of 0.69 and 0.68 is achieved for *S. anglia* using standardized data, but those values are 0 for *S. Inter media.*

In summary, the hierarchical clustering technique gives low accuracy and inconsistent precision and sensitivity across the species and classes.

5.3 Decision Tree
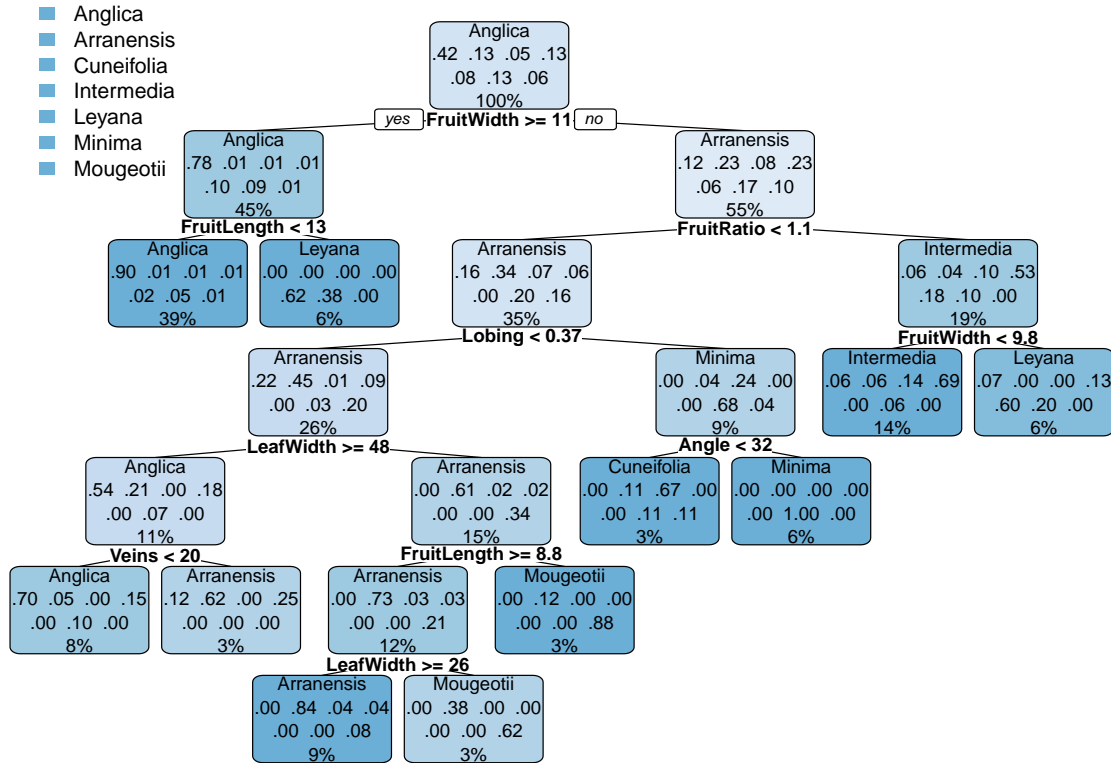
Figure 5: Decision tree

Table 4: Accuracy of the decision tree

0.68

Table 5: Confusion matrix for the decision tree

	Anglica	Arranensis	Cuneifolia	Intermedia	Leyana	Minima	Mougeotii	
Anglica	41	3	0	0	3	0	1	48
Arranensis	4	7	0	0	1	0	3	15
Cuneifolia	0	1	1	4	0	0	0	6
Intermedia	2	0	1	10	1	0	0	14
Leyana	3	0	0	0	6	0	0	9
Minima	1	0	0	1	4	9	0	15
Mougeotii	1	3	0	0	0	0	3	7

Table 16 of Appendix III shows numbers of species in each group, it is useful to be aware of the proportion of species in the test set when analyzing the tree plot.

The plot shows the decisions on which the tree has been split. The percentage is the percentage of

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observations in that leaf or node. The leaves represent the predicted class into which the data is split. The numbers in the leaves and the nodes show the predicted probability for each class.

The plot shows that the first decision splits the data roughly in half depending on the fruit being either greater or less than 11mm wide. The thinner fruit is then predominantly assigned to *S. anglica* based on the length being less than 13mm. The wider fruits take more decisions to assign the species. Fruit ratio (fruit width/fruit length) and fruit length < 9.8mm gives 14% of the data, most of which is allocated to *S.intermedia* with some *S. cuneifolia*. The *S. minima* leaf contains only that species (high precision) but only 6% of the data instead of 13% so we can see that around half this species has been incorrectly assigned (low sensitivity).

The accuracy of the tree, shown in table 4, is 0.68. The confusion matrix in table 5 shows that most of *S. anglica, S. intermedia, S.leyana*, and {*S.minima* are grouped together. The sensitivity and precision shown in tables 17 and 18 of Appendix III, demonstrate sensitivity above 0.6 for 5 out of the 7 species while precision is above 0.5 for 5 classes and 100% for *S. minima*.

5.4 Summary

A summary of precision and sensitivity for hierarchical clustering and the decision tree are shown in tables 6 and 7. The K-means has not been included since the inconsistency of the method demonstrates that it is not suitable for this data.

Table 6: Sensitivity for hierarchical clustering and decision tree

	hclust standardised	hclust non-standardized	tree
Anglica	0.68	0.32	0.85
Cuneifolia	0.28	0.04	0.47
Intermedia	0	0	0.17
Leyana	0.46	0.21	0.71
Minima	0	0.27	0.67
Mougeotii	0.06	0.04	0.6
Arranensis	0.48	0.87	0.43

Table 7: Precision for hierarchical clustering and decision tree

	hclust standardised	hclust non-standardized	tree
Class1	0.69	0.81	0.79
Class2	0.08	0.17	0.5
Class3	0	0	0.5
Class4	0.04	0.37	0.67
Class5	0.05	0	0.4
Class6	0.05	0.43	1
Class7	0.58	0.61	0.43

The decision tree is the most successful of the algorithms achieving the highest accuracy of 0.68, with precision and sensitivity being consistently higher across the classes and species.

6 Conclusion.

K-means was not successful in separating the data into clusters which could be interpreted as species of *Sorbus*. The algorithm was seen to be unrepeatable and the accuracy was always less 0.3. Sometimes high precision or sensitivity was achieved for a single species, but this was not reflected in the other species and it was not repeatable. The standardized data gave only slightly better results. It is not clear from this analysis whether it is the nature of the data itself that is the cause of the poor performance of this technique; Raykov et al (Raykov et al. 2016) describe the need for data subsets of equal variance and size, which was not the case here. Or the data preparation may have been at fault. Different methods of standardization have been shown to influence the outcome of K-means, and the method used here may not be the optimum, (Banks et al. 2011).

Hierarchical clustering achieved an accuracy of 0.42 using the Canberra method in non-standardized data and 0.41 using the Euclidean and Minowski method in standardized data. The sensitivity and precision demonstrated inconsistent results for the standardized and non-standardized data. Neither data treatment being better for all species. Overall, hierarchical clustering was not successful, and again, it is not clear whether this is due to the data preparation of the nature of the data. The fact that the non-standardized data sometimes gave better results is unexpected and has not been addressed.

The decision tree method performed more consistently than hierarchical clustering. Although a single species might have a higher sensitivity in clustering, across all species the decision tree performed better, with four of the seven species achieving greater than 0.6 sensitivity and precision above 0.5 in five of seven classes. The overall accuracy was also the highest at 0.68.

In conclusion, machine learning using a decision tree algorithm was a successful method for identifying species of *Sorbus*.

7 Further work

Different methods of standardization could be tried for the unsupervised methods, as well as other clustering algorithms which may be better able to model this data.

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All the variables were used in the decision tree, which may not be the best model. Rpart provides information on the importance of variables which can be used to ascertain which can be removed, and this might further improve performance.

The decision tree could be extended to include cross fold validation in order to give more robust predictions. Other species of *Sorbus* could be modeled to see if the success was due to the specific morphological characteristics of the *Soraria* subgenus and compare results for other subgenera.

Sorbus are particularly difficult to identify due to the similarity between species. It would therefore be interesting to use this model to asses more easily differentiated plants, such as grasses or sedges. These can be problematic to recorders due to the number of features that must be cross-referenced, but these features are more differentiated than in *Sorbus*.

Appendix I K-means results.

Table 8: Precision of kmeans with non standardized data

	1	2	3	4	5	6	7	8	9	10
Anglica	0.13	0.3	0.21	0.12	0.24	0.13	0.29	0.15	0.13	0.03
Cuneifolia	0	0.34	0.34	0.04	0	0.08	0.3	0.08	0.06	0.3
Intermedia	0.05	0.21	0	0.21	0.05	0.63	0.53	0	0.58	0
Leyana	0.06	0.17	0.06	0.06	0.21	0.06	0.02	0.02	0.06	0.29
Minima	0.07	0.3	0.03	0.03	0.03	0.1	0.23	0.03	0.37	0.37
Mougeotii	0.5	0.32	0.04	0.06	0.06	0.04	0.08	0.08	0.08	0.04
Arranensis	0	0	0.04	0	0.04	0	0.04	0	0	0

Table 9: Precision of kmeans with standardized data

	1	2	3	4	5	6	7	8	9	10
Anglica	0.02	0.02	0	0	0.53	0.18	0.49	0	0	0.28
Cuneifolia	0.02	0	0.06	0.46	0	0.06	0.48	0.34	0	0.1
Intermedia	0	0	0	0	0.05	0	0.95	0	0	0
Leyana	0.06	0	0.04	0.19	0	0.04	0.06	0.04	0.19	0.08
Minima	0	0	0	0.07	0	0	0	0.03	0	0
Mougeotii	0	0.06	0	0.06	0.06	0	0.06	0.06	0	0
Arranensis	0	1	1	0	1	0	0	0	0	0

Table 10: Sensitivity of kmeans with non standardized data

	1	2	3	4	5	6	7	8	9	10
Anglica	0.13	0.3	0.21	0.12	0.24	0.13	0.29	0.15	0.13	0.03
Cuneifolia	0	0.34	0.34	0.04	0	0.08	0.3	0.08	0.06	0.3
Intermedia	0.05	0.21	0	0.21	0.05	0.63	0.53	0	0.58	0
Leyana	0.06	0.17	0.06	0.06	0.21	0.06	0.02	0.02	0.06	0.29
Minima	0.07	0.3	0.03	0.03	0.03	0.1	0.23	0.03	0.37	0.37
Mougeotii	0.5	0.32	0.04	0.06	0.06	0.04	0.08	0.08	0.08	0.04
Arranensis	0	0	0.04	0	0.04	0	0.04	0	0	0

Table 11: Sensitivity of kmeans with standardized data

	1	2	3	4	5	6	7	8	9	10
Anglica	0.02	0.02	0	0	0.53	0.18	0.49	0	0	0.28
Cuneifolia	0.02	0	0.06	0.46	0	0.06	0.48	0.34	0	0.1
Intermedia	0	0	0	0	0.05	0	0.95	0	0	0
Leyana	0.06	0	0.04	0.19	0	0.04	0.06	0.04	0.19	0.08
Minima	0	0	0	0.07	0	0	0	0.03	0	0
Mougeotii	0	0.06	0	0.06	0.06	0	0.06	0.06	0	0
Arranensis	0	1	1	0	1	0	0	0	0	0

Appendix II Hierachical clustering results

Table 12: Accuracy obtained in hierarchical clustering using different distance metrics for standardized data

Distance Method	euclidean	maximum	manhattan	canberra	minkowski
Accuracy	0.41	0.14	0.36	0.25	0.41

Table 13: Confusion matrix for standardized data

	1	2	3	4	5	6	7
Anglica	52	17	27	6	10	43	5
Arranensis	5	2	2	12	1	1	27
Cuneifolia	0	0	0	1	0	0	18
Intermedia	6	2	0	10	0	7	23
Leyana	1	2	0	14	8	1	4
Minima	0	2	12	12	13	2	9
Mougeotii	0	0	0	3	0	0	20

Table 14: Precision for standardized and non-standardized data

	Standardized	Unstandardized
Class1	0.69	0.81
Class2	0.08	0.17
Class3	0	0
Class4	0.04	0.37
Class5	0.05	0
Class6	0.05	0.43
Class7	0.58	0.61

Table 15: Sensitivity for standardized and non-standardized data

	Standardized	Non-standardized
Anglica	0.68	0.32
Cuneifolia	0.28	0.04
Intermedia	0	0
Leyana	0.46	0.21
Minima	0	0.27
Mougeotii	0.06	0.04
Arranensis	0.48	0.87

Appendix III Decision tree results

Table 16: Proportions of each species in test set

Anglica	0.42
Arranensis	0.13
Cuneifolia	0.05
Intermedia	0.13
Leyana	0.08
Minima	0.13
Mougeotii	0.06

Table 17: Sensitivity for the decision tree

Species	Sensitivity
Anglica	0.85
Arranensis	0.47
Cuneifolia	0.17
Intermedia	0.71
Leyana	0.67
Minima	0.6
Mougeotii	0.43

Table 18: Precision for the decision tree

Class	Precision
class_Anglica	0.79
class_Arranensis	0.5
class_Cuneifolia	0.5
class_Intermedia	0.67
class_Leyana	0.4
class_Minima	1
class_Mougeotii	0.43

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