Group 13 Contributions: Shenghua Zhu, Truell Clark, Anish Ravilla

All three of us helped write the data acquisition and preparation, with Isaac leading us in this process with guidance and advice. Isaac helped create the box plots, the correlation heatmap, and the feature selection chart, along with the implementation of a Random Forest Classifier. Isaac also programmed the decision boundary function. Anish helped create the groupby chart, the hisograms of the physical features for each penguin species, the function to visualize confusion matrices, and the implementation of a Logistic Regression model with its respective confunsion matrix and decision boundary plot. Truell contributed the majority of the written explanations for the explanatory data analysis and the implementation of the K-Nearest machine learning model, along with its respective confusion matrix and decision boundary plot.

Project: How can we use Machine Learning Models to Predict the Species of a Penguin?

For this project, our goal is to determine which variables are the most predictive of a penguin's species. We are using the Palmer Penguins data set, which was collected by Dr. Kristen Gorman. To efficiently and concisely build a model that can accomplish our task, we download the following libraries. Matplotlib and seaborn are used for the display of our data, while the rest of the libraries help clean, process, and examine the data.

```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn import preprocessing
```

Data Import and Cleaning

Next, we store the Palmer Penguins data under an easy-to-access variable called penguins and look at the structure of our data.

Data	columns (total 17 columns):									
#	Column	Non-Null Count Dtype								
0	studyName	344 non-null	object							
1	Sample Number	344 non-null	int64							
2	Species	344 non-null	object							
3	Region	344 non-null	object							
4	Island	344 non-null	object							
5	Stage	344 non-null	object							
6	Individual ID	344 non-null	object							
7	Clutch Completion	344 non-null	object							
8	Date Egg	344 non-null	object							
9	Culmen Length (mm)	342 non-null	float64							
10	Culmen Depth (mm)	342 non-null	float64							
11	Flipper Length (mm)	342 non-null	float64							
12	Body Mass (g)	342 non-null	float64							
13	Sex	334 non-null	object							
14	Delta 15 N (o/oo)	330 non-null	float64							
15	Delta 13 C (o/oo)	331 non-null	float64							
16	Comments	26 non-null	object							
<pre>dtypes: float64(6), int64(1), object(10)</pre>										
memory usage: 45.8+ KB										
None										

We ran a df.unique() method for the certain variables to make sure that there was variation between the variables for us to analyze. For instance, if there was only one unique value, such as for the "Region" variable, we removed it from our model. In our search for variables that are predictive of species, variables that are the same for each penguin will not be helpful.

Then we check for NA values in our training and testing sets

```
X_train.isna().sum()
    Island
    Culmen Length (mm)
    Clutch Completion
    Culmen Depth (mm)
    Flipper Length (mm)
                             1
    Body Mass (g)
                             1
    Sex
                             8
    Delta 15 N (o/oo)
                            11
    Delta 13 C (o/oo)
                            10
    dtype: int64
```

```
X test.isna().sum()
     Island
                             0
     Culmen Length (mm)
    Clutch Completion
                             0
    Culmen Depth (mm)
                             1
    Flipper Length (mm)
                             1
                             1
    Body Mass (q)
                             2
     Sex
                             3
    Delta 15 N (o/oo)
    Delta 13 C (o/oo)
                             3
    dtype: int64
y train.isna().sum()
     0
y test.isna().sum()
     0
```

Create data preprocessing pipelines for cleaning and labeling.

```
def clean(df):
  df = df.dropna()
  df = df[df['Sex']!='.']
  return df
def label(df):
  df = pd.DataFrame(df)
  le = preprocessing.LabelEncoder()
  df = df.apply(le.fit transform)
  return df
X = label(X)
y = label(y)
X train = label(clean(X train))
X_test = label(clean(X_test))
y train = label(y train)
y test = label(y test)
#check x train
X train.head()
```

Culmen Clutch
Island Length Completion Culmen Flipper Body Delta Delta

Opposition Depth Length Mass Sex 15 N 13 C

After data cleaning and labeling, we can see that X_train and X_test is free of NA values and all the categorical variables are encoded as integer values. We mark the indices of penguins that we dropped from X_train and X_test and drop the corresponding species in y_train and y_test to make sure that our training and testing sets match in size.

```
new_train_index = [index for index in X_train.index if index in y_train.index]
y_train = y_train.loc[new_train_index]
new_test_index = [index for index in X_test.index if index in y_test.index]
y_test = y_test.loc[new_test_index]
X_train.shape,X_test.shape,y_train.shape,y_test.shape

((225, 9), (99, 9), (225, 1), (99, 1))
```

Exploratory Data Analysis

We first check the distrbution of the penguins species

```
penguins["Species"].value_counts(normalize=True)
#0: Adelie Penguin
#1: Chinstrap penguin
#2: Gentoo penguin

Adelie Penguin (Pygoscelis adeliae) 0.441860
Gentoo penguin (Pygoscelis papua) 0.360465
Chinstrap penguin (Pygoscelis antarctica) 0.197674
Name: Species, dtype: float64
```

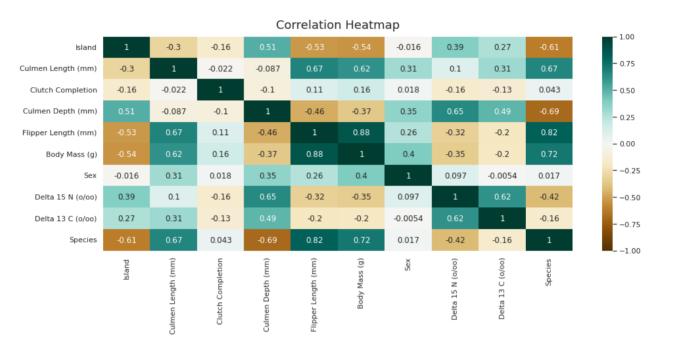
Based on the penguins data, we have 44.2% of Adelie Penguin, 36.0% of Chinstrap Penguin, and 19.8% of Gentoo Penguin.

```
#We combine the training and testing data to produce a clean penguins dataframe for
train = pd.concat([X_train,y_train],axis=1)
test = pd.concat([X_test,y_test],axis=1)
new_penguins = pd.concat([train,test],axis=0)
```

One of the first steps we take in our exploratory analysis is to create a correlation heatmap. The grid below displays the correlation between all variables in our dataframe. Positive values indicate a positive relationship between two variables, with 1 being a perfect positive relationship, and negative values indicating a negative relationship. A value of 0 is interpreted as there being no correlation between two variables. For modeling purposes, we focus on variables

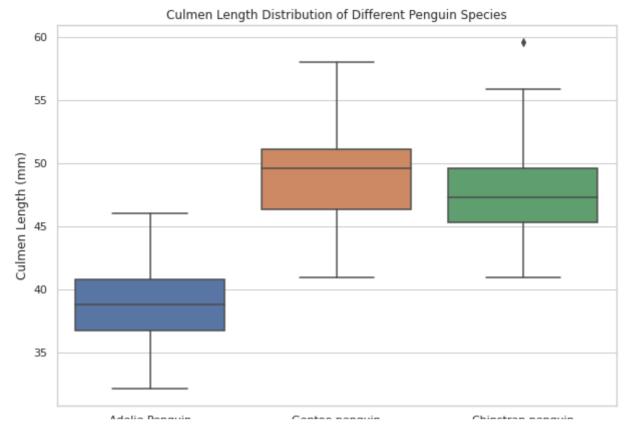
that have correlations with species that are of large magnitude. A strong positive or negative correlation shows that variables may be useful in predicting each other.

```
#Correlation Heatmap
plt.figure(figsize=(16, 6))
heatmap = sns.heatmap(new_penguins.corr(), vmin=-1, vmax=1, annot=True, cmap='BrBG'
heatmap.set_title('Correlation Heatmap', fontdict={'fontsize':18}, pad=12)
plt.show()
```



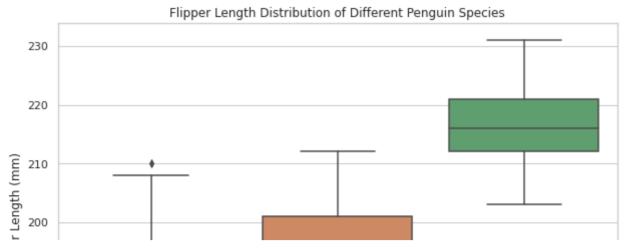
As stated above, we are interested in variables that have high a correlation with the Species variable. These include *Culmen Length*, *Flipper Length*, *Body Mass*, *and Island*. From these variables we are going to choose **2 features** and **1 qualitative feature**. In the next section, we'll explore the distribution of these significant variables to see if they can be included in our model.

```
fig = plt.figure(figsize =(10, 7))
sns.set_theme(style="whitegrid")
sns.boxplot(x="Species", y="Culmen Length (mm)", data= penguins)
plt.xticks([0, 1, 2], ['Adelie Penguin', 'Gentoo penguin', 'Chinstrap penguin'])
plt.title('Culmen Length Distribution of Different Penguin Species')
plt.show()
```



Here, we created a figure that displays a boxplot for the Culmen Length distribution for each species. From the figure, we see that the Adelie penguins have comparatively shorter Culmen Lengths, as 50% of the data lie between approximately 36 and 41mm. Chinstrap and Gentoo penguins have much more similar distributions, as 50% of the data of both penguins lie between approximately 45 and 51mm. We also see that nearly all penguins with Culmen Length less than 41mm are Adelie penguins, and that approximately 75% of Adelie penguins have Culmen Lengths less than 41mm. From this we assume that Culmen Length will be very helpful in identifying the majority of Adelie penguins, but not very helpful in distinguishing Gentoo penguins from Chinstrap.

```
fig = plt.figure(figsize =(10, 7))
sns.set_theme(style="whitegrid")
sns.boxplot(x="Species", y="Flipper Length (mm)", data= penguins)
plt.xticks([0, 1, 2], ['Adelie Penguin', 'Gentoo penguin', 'Chinstrap penguin'])
plt.title('Flipper Length Distribution of Different Penguin Species')
plt.show()
```

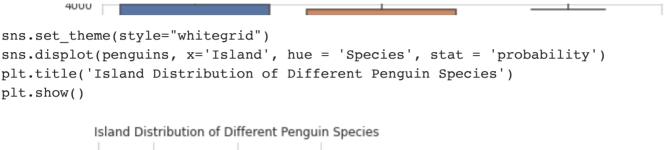


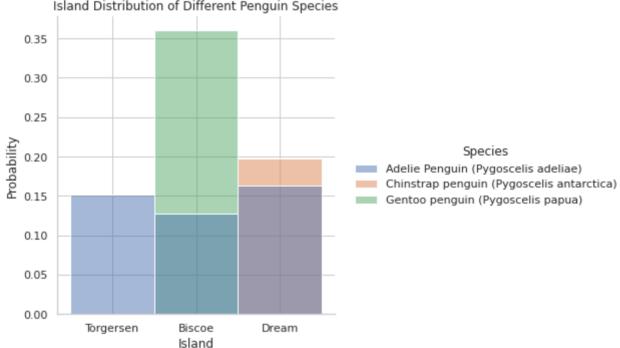
Additionally, we created a boxplot figure for the Flipper Length distribution for each species. From the plot, we observe that Chinstrap penguins have much longer Flipper Lengths than both Gentoo and Adelie penguins. The median Flipper Length for the Chinstrap penguins is approximately 216mm, while the medians of Gentoo and Adelie penguins are approximately 190 and 196mm. Furthermore, 75% of Chinstrap penguins have Flipper Lengths greater than 212mm, and that there is not a single Gentoo and Adelie penguin with Flipper Lengths longer than this. Flipper Length is very helpful in distinguishing Chinstrap penguins from the other two species, but will not be as useful for differentiating Gentoo penguins from Adelie.

```
fig = plt.figure(figsize =(10, 7))
sns.set_theme(style="whitegrid")
sns.boxplot(x="Species", y="Body Mass (g)", data= penguins)
plt.xticks([0, 1, 2], ['Adelie Penguin', 'Gentoo penguin', 'Chinstrap penguin'])
plt.title('Body Mass Distribution of Different Penguin Species')
plt.show()
```

Body Mass Distribution of Different Penguin Species

Above, our final box plot displays the Body Mass distribution for each species. Here, we see that the distribution for the Chinstrap penguins once again sticks out amongst the others. The median Body Mass for a Chinstrap penguin is approximately 5000g, while Adelie and Gentoo penguins have very similar medians that are both approximately 3700g. At least 50% of Chinstrap penguins have body mass greater than 4900g, and neither the Adelie nor the Gentoo penguin groups contain a penguin with Body Mass this large. Similar to Flipper Length, Body Mass greatly helps to distinguish Chinstrap penguins for the other two species, but does not help to distinguish Gentoo and Adelie penguins from each other.





Above is a stacked bar plot of the island distribution of different penguin species. Adelie penguins are the only species present on all three islands, while chinstrap penguins and gentoo penguins are on Biscoe and Dream island respectively. Approximately 35% of Biscoe Island consists of Gentoo penguins, the highest proportion of a single penguin species out of any island.

Below is a table display of some summary statistics of the variables that we wish to analyze as predictor variables. We chose the variables of Culmen Length, Flipper Length, and Body Mass, as these are the variables with the highest correlations with Species, as seen in the heat map above. We breakdown the variables by species and calculate the mean, standard deviation,

minimum, and maximum for each variable based on the species. In the species column, 0 corresponds with Adelie, 1 corresponds with Chinstrap, and 2 corresponds with Gentoo. In the island column, 0 corresponds with Dream, 1 corresponds with Biscoe, and 2 corresponds with Torgersen.

```
#Variables we wish to analyze as possible predictor variables
cols = ['Culmen Length (mm)', 'Flipper Length (mm)', 'Body Mass (g)' ]
train.groupby(["Species", "Island"])[cols].aggregate([np.mean, np.std, np.min, np.m
```

		Culmen Length (mm)				Flipper Length (mm)			
		mean	std	amin	amax	mean	std	amin	am
Species	Island								
0	0	31.033333	16.325321	4	76	11.700000	5.995113	0	
	1	28.815789	16.531469	0	66	13.789474	6.485568	3	
	2	30.200000	18.823744	2	66	16.960000	6.483826	2	
1	1	102.468085	24.583355	44	136	20.042553	6.733942	5	
2	0	90.317647	21.879111	44	137	38.941176	5.780412	29	

In order to gain a sense of what the distributions for these high correlation variables look like, we created a histogram that distinguishes between each species for each of these variables, with the use of the groupby and apply functions.

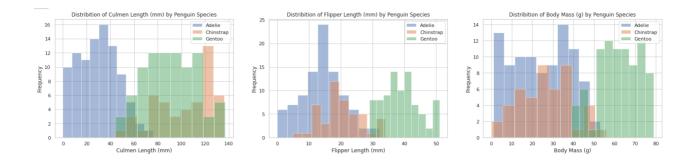
```
cols = ['Culmen Length (mm)', 'Flipper Length (mm)', 'Body Mass (g)']

fig, ax = plt.subplots(1,len(cols), figsize = (25,5)) #Initialize plot

def plot_hist(train, cols, alpha):
    '''
    This function iterates through a list of chosen variables and plots histograms for each of these variables based on the different penguin species.
    '''
    for i in range(len(cols)):
        ax[i].hist(train[cols[i]], alpha = alpha) #Plot histogram
        ax[i].set(title = "Distribition of " + cols[i] + " by Penguin Species")
        ax[i].set(ylabel = "Frequency")
        ax[i].set(xlabel = cols[i])

    #Create legend
    labels = ["Adelie", "Chinstrap", "Gentoo"]
        ax[i].legend(labels)
```

#Use groubpy to plot histograms for each species
train.groupby("Species").apply(plot hist, cols, 0.5)



In the culmen length histogram, we see that Adelie penguins are on the lower end of the distribution while gentoo and chinstrap penguins are higher up. The adelie penguin distribution is skewed to the left, the chinstrap distribution is skewed to the right, and the gentoo distribution is almost symmetrical.

In the flipper length histogram, we see that adelie penguins make up the mimimum flipper length, while gentoo penguins make up the maximum length. All of the distributions are relatively symmetrical. An interesting thing to note here is that there is a high prevalence of adelie penguins with a length of around 12 mm.

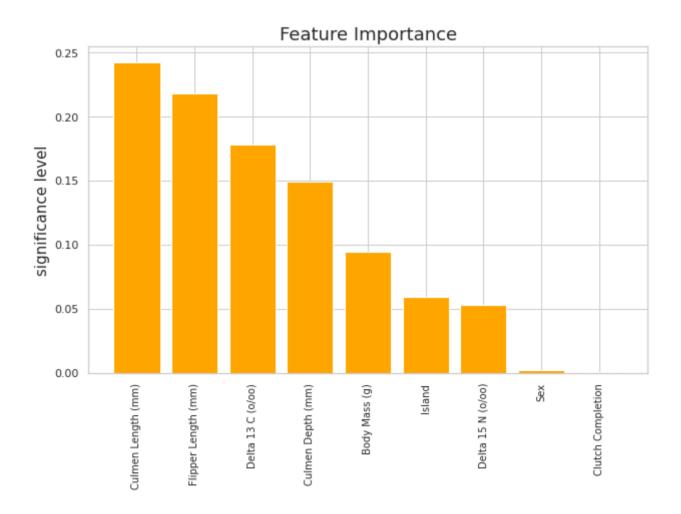
In the body mass histogram,, we also see distributions that are approximately symmetrical for each penguin species. Chinstrap and adelie penguins make up the lower end of the spectrum, while the maximum penguin masses exclusively consist of gentoo penguins. Gentoo penguins seem to be the most physically imposing penguin species from these physical features.

Feature Selection

In our exploratory analysis, we use a correlation heatmap to filter variables that we believe are important, which are Culmen Length, Flipper Length, Body Mass, and Island. In this section, we are going to use **random forest classification to help validate our choice of features**. In general, feature selection using Random forest gives a good predictive performance, low overfitting, and

easy interpretability. Basically, we compute how much each variable is contributing to the decision and calculate their feature importance.

```
= ['Island', 'Culmen Length (mm)', 'Clutch Completion', 'Culmen Depth (mm)',
features
              'Flipper Length (mm)', 'Body Mass (g)', 'Sex', 'Delta 15 N (o/oo)', 'Delt
forest = RandomForestClassifier(n estimators=1000, random state=0, n jobs=-1)
forest.fit(X train, y train)
importances = forest.feature importances
indices = np.argsort(importances)[::-1]
order=[]
for x in range(X_train.shape[1]):
    order.append(features[indices[x]])
plt.figure(figsize=(10,6))
plt.title("Feature Importance", fontsize = 18)
plt.ylabel("significance level", fontsize = 15, rotation=90)
for i in range(len(features)):
   plt.bar(i,importances[indices[i]],color='orange',align='center')
    plt.xticks(np.array([*range(len(features))]),order,rotation=90,fontsize=10)
plt.show()
```



In the feature importance plot, we sort the variables in terms of their feature importance in descending order. The two quantitative features with the greatest importance are Culmen Length

and Flipper Length, and the qualitative feature with the greatest importance is Island. This result agrees with what we obtained from the correlation heatmap. Therefore, for our feature selection, we'll use **Culmen Length**, **Flipper Length**, **and Island**.

Modeling

```
from sklearn.linear model import LogisticRegression
from sklearn.model selection import cross val score
from sklearn.ensemble import RandomForestClassifier
from sklearn.model selection import RepeatedStratifiedKFold
from sklearn import metrics
from sklearn.metrics import accuracy score, confusion matrix, classification report
from matplotlib.colors import LinearSegmentedColormap
from sklearn.neighbors import KNeighborsClassifier
import warnings
#Subset the wanted predictor variables from the X train dataset
Features = ['Culmen Length (mm)','Flipper Length (mm)','Island']
X train new = X train[Features]
X test new = X test[Features]
#Note: Data has already been cleaned so no need to clean again
#Keep track of the categorical variables
#0: Adelie Penguin
#1: Chinstrap penguin
#2: Gentoo penguin
#0: Biscoe
#1: Dream
#2: Torgersen
list(set(penguins['Island']))
    ['Dream', 'Torgersen', 'Biscoe']
def plot decision boundary(model):
  qualitative fts names = list(set(penguins['Island']))
  qualitative fts names.sort()
  qualitative fts = list(set(X['Island']))
  species names = ['Adelie','Chinstrap','Gentoo']
  species_col = ['red','green','blue']
  masks = []
  for i in range(len(qualitative fts)):
    masks.append(X['Island'] == qualitative fts[i])
  for i in range(len(masks)):
    xi = X[masks[i]]
    x0 = xi[Features[0]]
    x1 = xi[Features[1]]
```

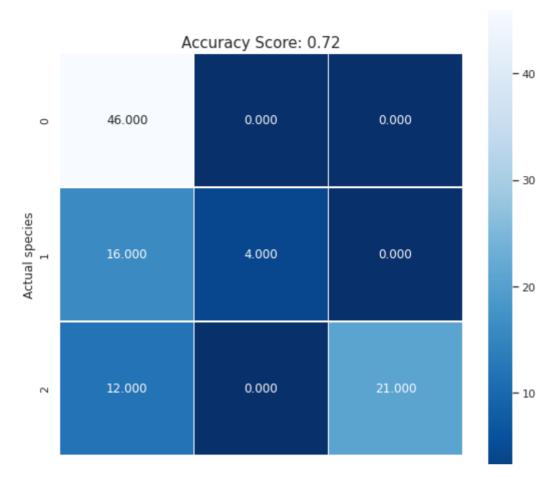
```
yi = y['Species'][masks[i]]
grid x = np.linspace(x0.min(), x0.max(), 501)
grid y = np.linspace(x1.min(),x1.max(),501)
z = qualitative fts[i]*np.ones(501*501)
xx,yy = np.meshqrid(qrid x,qrid y)
XX = xx.ravel()
YY = yy.ravel()
zz = z.ravel()
p = model.predict(pd.DataFrame(np.c_[XX,YY,ZZ],columns=Features))
p values = list(set(p))
yi values = list(set(yi))
color list region = []
color list scatter = []
for j in range(len(p values)):
  color_list_region.append(species_col[p_values[j]])
for k in range(len(yi values)):
  color_list_scatter.append(species_col[yi_values[k]])
self cmap region = LinearSegmentedColormap.from list('mycmap',color list region
self cmap scatter = LinearSegmentedColormap.from list('mycmap',color list scatt
p=p.reshape(xx.shape)
fig,ax = plt.subplots(1)
ax.contourf(xx,yy,p,cmap=self cmap region,alpha=.2)
for s in range(len(yi values)):
  maskl = yi==yi values[s]
  ax.scatter(x0[maskl], x1[maskl], color=species_col[yi_values[s]], label=speci
  #set the title and label our axis
  ax.set(title="Island"+': '+ qualitative fts names[i])
  ax.set(xlabel = Features[0], ylabel = Features[1])
  ax.legend()
```

MODEL 1: Logistic Regression

Now we are going to construct a machine learning model to try and judge how accurate each predictor variable is in predicting the species of the penguin. Below we will implement a logistic regression model in order to discern if there is a relationship between each of the variables with the encoded species values. We extracted the two top quantitative variables from the feature selection bar graph above along with the top qualititative variable to use as predictor variables.

```
np.random.seed(1234)
#Now perform cross validation testing
# 10-fold cross validation: hold out 10%, train on the 90%, repeat 10 times.
#Output accuracy scores for each 10-fold cross validation
```

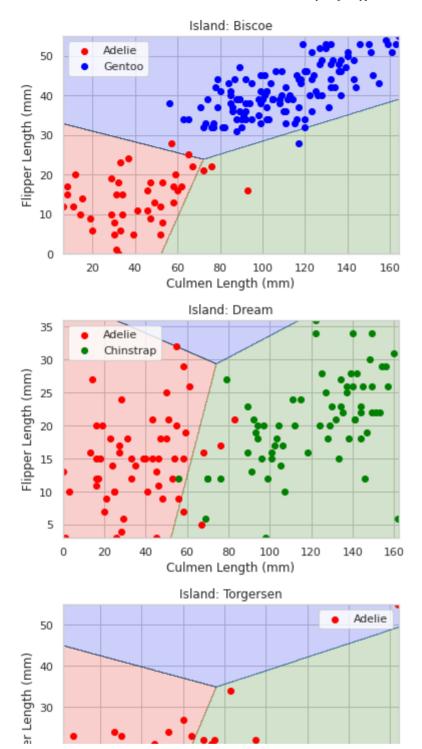
```
#cv scores = cross val score(train model, X train, y train, cv=10)
c values = np.linspace(0.1, 5, num = 50)
best mean = 0
best c = 0
best model = LogisticRegression(C = 0.1).fit(X train new, y train)
for c in c values:
   warnings.filterwarnings("ignore")
   model = LogisticRegression(C = c).fit(X train new, y train)
   cv score = cross val score(model, X train new, y train, cv = 10).mean()
    if cv score >= best mean:
        best mean = cv score
        best c = c
        best model = model
predictions = best model.predict(X test new)
training score = round(best model.score(X train new, y train), 2)
score = round(best model.score(X test new, y test), 2)
print('Test Score Accuracy: %.3f'% score)
print("Training Score Accuracy = " + str(training_score))
    Test Score Accuracy: 0.720
    Training Score Accuracy = 0.98
from sklearn.metrics import confusion matrix
from sklearn.metrics import plot confusion matrix
import matplotlib.pyplot as plt
import seaborn as sns
#Function to plot confusion matrices for different models
def cm generator(cm, score):
 plt.figure(figsize=(9,9))
 sns.heatmap(cm, annot=True, fmt=".3f", linewidths=.5, square = True, cmap = 'Blue
 plt.ylabel('Actual species');
 plt.xlabel('Predicted species');
 all sample title = 'Accuracy Score: {0}'.format(score)
 plt.title(all sample title, size = 15);
cm = confusion matrix(y test, predictions, labels = [0, 1, 2])
cm generator(cm, score)
```



This mean accuracy score gives us an overall picture of how well we can expect the regression model we developed to perform against actual test data. We used a k-value of 10 (data split into ten groups) as this is the value that generally limits bias between the training and test data. We then iterated over a different complexity parameter and chose the best logistic regression model - which corresponded with the model that contained the best mean cross validation scores from the different folds.

We used this model to predict the test results and compared them to the actual test results we split from the data. The confusion matrix above indicates how accurate our model was in predicting the species based on the variables we chose. The values on the diagonal correspond with matrix values (i,j) where i = j. So for instance, the model accurately predicted 46 penguins in the test set to be Adelie penguins (species 0). The numbers off the diagonal correspond to the number of species the model predicted incorrectly. For example, the number incorrectly predicted 16 Adelie penguins when these penguins were actually Chinstrap penguins. As a result, the model was only 72% accurate.

plot decision boundary(best model)



This decision boundary plot allows us to visualize how this logistic regression model arrived at its predictions. Correct predictions of the model are identified with points that match up in the zone that corresponds with the same color. For instance, the model correctly predicted Adelie penguins if the red points corresponding to Adelie penguins matched up to the red zone in the plot. Overall, the model generally predicted the correct penguin species, although it predicted 38 chinstrap and gentoo penguins as adelie penguins perhaps due to its prevalence on every island. Perhaps the machine learning model is equally weighing the importance of the categorical variable of island to the two quantitative variables of flipper Length and culmen Length, although our feature selection shows that flipper length and culmen length should have more influence in determining the penguin species. If the island is given equal weight, then it would have more

influence than we expect it to, hence the over-prediction of other penguin species as adelie

MODEL 2: Random Forest

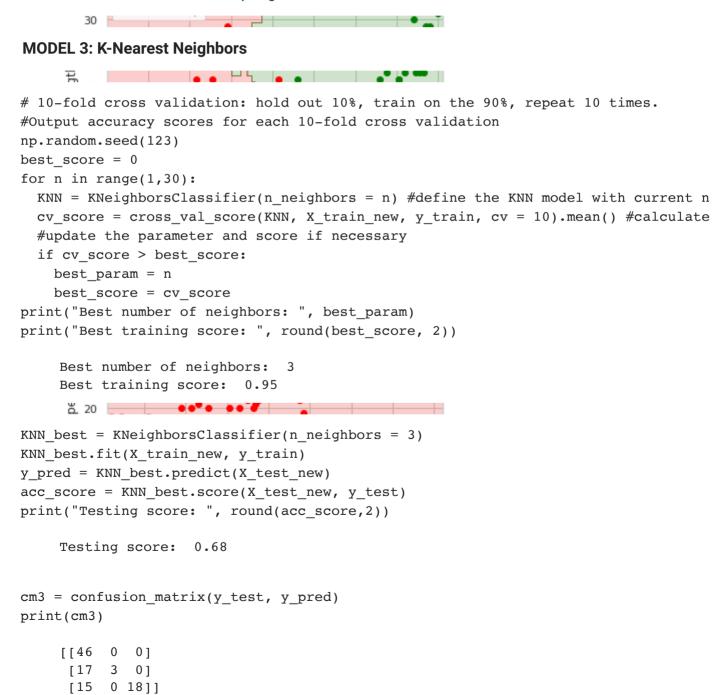
```
#Now perform cross validation testing
# 10-fold cross validation: hold out 10%, train on the 90%, repeat 10 times.
#Output accuracy scores for each 10-fold cross validation
np.random.seed(123)
best cv score = 0
scores=np.zeros(30)
for i in range (1, 30+1):
 clf = RandomForestClassifier(n estimators = i)
 scores[i-1] = cross val score(clf, X train new, y train, cv = 10).mean() #Update
 if scores[i-1] > best cv score:
       best n estimator = i
       best cv score = scores[i-1]
       clf best = clf.fit(X train new, y train)
       best testing score = clf.score(X test new, y test)
y pred = clf best.predict(X test new)
print("Best n estimators: " + str(best n estimator))
print("Best Training Score: " + str(round(best cv score,2)))
print("Best Testing score: " + str(round(best testing score, 2)))
    Best n estimators: 10
    Best Training Score: 0.98
    Best Testing score: 0.72
#create confusion matrix
cm2 = confusion_matrix(y_test, y_pred)
print(cm2)
    [[46 0 0]
     [14 6 0]
     [14 0 19]]
#Visual Display of confusion matrix
cm generator(cm2, round(best testing score,2))
```



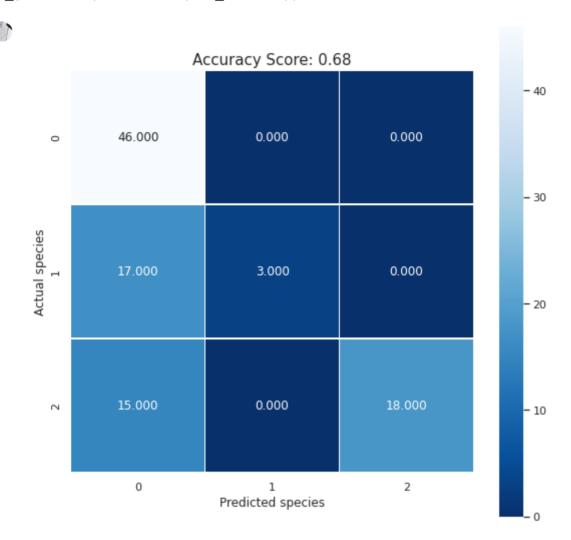
plot_decision_boundary(clf_best)



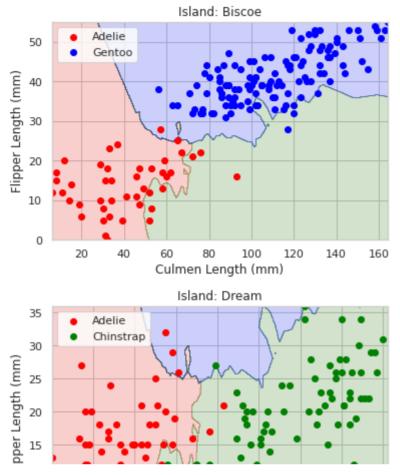
This decision boundary plot allows us to visualize how the random forest model classified the data. Similar to the previous decision boundary plot, correct predictions are indicated with points matching the color of the region. This model was most accurate for classification of penguins on the Biscoe Island, as it only misclassified one Adelie penguin as Gentoo. The model was far less accurate for the Dream island. It correctly predicted all of the Chinstrap penguins on this island, but misclassified 8 of the Adelie penguins as Chinstrap. For Torgersen Island, the model similarly misclassified 2 Adelie penguins as Chinstrap. Overall, the model made very few classification mistakes outside of the Adelie penguins.



#Visual Display of confusion matrix
cm_generator(cm3, round(acc_score,2))



plot_decision_boundary(KNN_best)



This decision boundary plot allows us to visualize how the K-nearest model classified the data. This plot shows a major difference between this model and the other two, as there was a classification region for each of the species on every Island. On Biscoe Island, some of the Adelie and Gentoo penguins were misclassified as Chinstrap, even though there were no Chinstrap penguins on the island. Only one other mistake was made in the model, as an Adelie penguin was classified incorrectly as Gentoo. On Dream Island, the model misclassified several penguins as Gentoo, although no Gentoo penguins were on this island. Aside from this, the model misclassified 6 Adelie penguins as Chinstrap. On Torgersen Island, a few Adelie penguins were classified as Chinstrap and Gentoo penguins. In reality, this island only consisted of Adelie penguins.

Final Discussion:

We decided to choose the **Random Forest Classification model** due to its high accuracy score and its versatility, as the logistic regression really only works best on binary classification features, which we did not have. The accuracy score for the random forest model was **72**%, while the scores for our logistic regression and KNN models were 72% and 68% respectively. The reason for their relatively poor performance can be attributed to our feature selection. With hindsight, it may have been better to include **the sex** of the penguins as our categorical variable rather than the island, as the influence of the Island variable may have been responsible for some

of the classification error we saw in our machine learning model. The model could be improved by including Sex as one of our features in our model.

✓ 23s completed at 4:45 PM

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