Logistic Regression

Supervised machine learning to classify a bivariate categorical target variable.

In [1]:
```
import pandas as pd
import numpy as np
import random
import statsmodels.api as sm
import statsmodels.formula.api as smf
from statsmodels.stats.outliers_influence import variance_inflation_factor
from sklearn.metrics import accuracy_score
import seaborn as sns
import matplotlib.pyplot as plt
```

Dataset

This data contains information about the characteristics of Penguins collected by Dr. Kristen Gorman in the Palmer station in Antartica (https://github.com/allisonhorst/palmerpenguins/tree/main).

In [2]:
```
#load the data
df = pd.read_csv("https://raw.githubusercontent.com/dswede43/ML-methods/main/data/palmerpenguins.csv")
df = df.dropna() #remove NA values
df = df.reset_index(drop = True) #reset the index
df = df.apply(lambda x: pd.factorize(x)[0]) #convert categorical variables into binary
```

Objective

Create a logistic regression ML model to classify the sex of a penguin.

Train and test data splitting

In [3]:
```
#function to split the data into folds for cross-validation
def k_folds_split(df, k):
    #test set size
    test_size = len(df) // k

    #data frame indices
    df_idx = list(range(len(df))) #all indices
    unsampled_idx = df_idx #unsampled indices

    #split training and testing sets
    train_test_sets = []
    for _ in range(k):
        test_idx = random.sample(unsampled_idx, test_size) #test set indices
        train_idx = [x for x in df_idx if x not in test_idx] #train set indices
        unsampled_idx = [x for x in unsampled_idx if x not in test_idx] #update unsampled indices

        #create test and train sets based on indices
        test_df = df.iloc[test_idx]
        train_df = df.iloc[train_idx]
        train_test_sets.append([test_df, train_df])

    return train_test_sets
```

In [4]:
```
#split the data into folds for cross-validation
random.seed(42) #set seed
k = 10 #number of folds
train_test_sets = k_folds_split(df, k)

#look at the first set of test and train data
test_set = train_test_sets[0][0]
test_set = sm.add_constant(test_set) #add column of 1 for constants
train_set = train_test_sets[0][1]
train_set = sm.add_constant(train_set) #add column of 1 for constants
```

Model selection

Model selection using an initial set of train and test data to create the different logistic regression models that will be performance tested using 10-fold cross validation.

Full additive model

Model including all feature variables:

$$logit(sex) = \beta_0 + \beta_1 species + \beta_2 island + \beta_3 billlength + \beta_4 billdepth + \beta_5 flipperlength + \beta_6 bodymass + \epsilon$$

In [5]:
```
#define the model formula
model_formula = 'sex ~ species + island + bill_length_mm + bill_depth_mm + flipper_length_mm + body_mass_g'

#train the data using logisitic regression
full_add_model = smf.logit(formula = model_formula, data = train_set).fit()
full_add_model.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.631288
         Iterations 5
```

Out[5]:

Logit Regression Results

Dep. Variable:	sex	**No. Observations:**	300
Model:	Logit	**Df Residuals:**	293
Method:	MLE	**Df Model:**	6
Date:	Sat, 02 Mar 2024	**Pseudo R-squ.:**	0.08913
Time:	09:25:31	**Log-Likelihood:**	-189.39
converged:	True	**LL-Null:**	-207.92
Covariance Type:	nonrobust	**LLR p-value:**	1.713e-06

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	0.3350	0.380	0.881	0.378	-0.410	1.080
species	0.4856	0.282	1.724	0.085	-0.066	1.038
island	-0.0788	0.214	-0.369	0.712	-0.498	0.340
bill_length_mm	-0.0139	0.005	-2.675	0.007	-0.024	-0.004
bill_depth_mm	0.0411	0.009	4.677	0.000	0.024	0.058
flipper_length_mm	-0.0309	0.013	-2.410	0.016	-0.056	-0.006
body_mass_g	-0.0109	0.007	-1.638	0.101	-0.024	0.002

Checking for multicollinearity

In [6]:
```
#function to calculate VIF scores
def vif_scores(X_train):
    vif = pd.DataFrame()
    vif['vif'] = [variance_inflation_factor(X_train.values, X) for X in range(X_train.shape[1])]
    vif['feature'] = X_train.columns

    return vif
```

In [7]:
```
#define the feature variables
features = ['species',
            'island',
            'bill_length_mm',
            'bill_depth_mm',
            'flipper_length_mm',
            'body_mass_g']

#calculate the VIF scores for each feature
vif = vif_scores(train_set[features])
vif
```

Out[7]:

	vif	feature
0	5.241273	species
1	3.250769	island
2	11.867773	bill_length_mm
3	6.543099	bill_depth_mm
4	7.249836	flipper_length_mm
5	5.327354	body_mass_g

The features *bill_length_mm* and *flipper_length_mm* show evidence of multicollinearity given their high VIF scores.

In [8]:
```
#define the feature variables
features = ['species',
            'island',
            'bill_depth_mm',
            'body_mass_g']

#calculate the VIF scores for each feature
vif = vif_scores(train_set[features])
vif
```

Out[8]:

	vif	feature
0	2.887494	species
1	2.964468	island
2	4.715387	bill_depth_mm
3	3.736665	body_mass_g

The VIF scores are now below 5; therefore, there is no longer any issues with multicollinearity among feature variables.

Reduced additive model 1

Model with collinear feature variables removed.

$$logit(sex) = \beta_0 + \beta_1 species + \beta_2 island + \beta_3 billdepth + \beta_4 bodymass + \epsilon$$

In [9]:

```
#define the model formula
model_formula = 'sex ~ species + island + bill_depth_mm + body_mass_g'

#train the data using logisitic regression
red_add_model1 = smf.logit(formula = model_formula, data = train_set).fit()
red_add_model1.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.657444
         Iterations 5
```

Out[9]:

Logit Regression Results

Dep. Variable:	sex	**No. Observations:**	300
Model:	Logit	**Df Residuals:**	295
Method:	MLE	**Df Model:**	4
Date:	Sat, 02 Mar 2024	**Pseudo R-squ.:**	0.05139
Time:	09:25:31	**Log-Likelihood:**	-197.23
converged:	True	**LL-Null:**	-207.92
Covariance Type:	nonrobust	**LLR p-value:**	0.0002676

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	-0.0282	0.360	-0.078	0.937	-0.733	0.677
species	-0.1600	0.190	-0.844	0.399	-0.532	0.212
island	-0.0406	0.208	-0.195	0.845	-0.448	0.367
bill_depth_mm	0.0276	0.008	3.626	0.000	0.013	0.042
body_mass_g	-0.0231	0.006	-3.921	0.000	-0.035	-0.012

The features *species* and *island* are non-significant and therefore removed.

Reduced additive model 2

Model with non-significant feature variables removed.

$$logit(sex) = \beta_0 + \beta_1 billdepth + \beta_2 bodymass + \epsilon$$

In [10]:

```
#define the model formula
model_formula = 'sex ~ bill_depth_mm + body_mass_g'

#train the data using logisitic regression
red_add_model2 = smf.logit(formula = model_formula, data = train_set).fit()
red_add_model2.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.659409
         Iterations 5
```

Out[10]:

Logit Regression Results

Dep. Variable:	sex	**No. Observations:**	300
Model:	Logit	**Df Residuals:**	297
Method:	MLE	**Df Model:**	2
Date:	Sat, 02 Mar 2024	**Pseudo R-squ.:**	0.04855
Time:	09:25:31	**Log-Likelihood:**	-197.82
converged:	True	**LL-Null:**	-207.92
Covariance Type:	nonrobust	**LLR p-value:**	4.130e-05

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	-0.1462	0.240	-0.609	0.543	-0.617	0.325
bill_depth_mm	0.0258	0.007	3.586	0.000	0.012	0.040
body_mass_g	-0.0229	0.006	-3.935	0.000	-0.034	-0.012

Interaction model

Model with interaction terms.

$$logit(sex) = \beta_0 + \beta_1 billdepth + \beta_2 bodymass + \beta_3 billdepth * bodymass + \epsilon$$

In [11]:

```
#define the model formula
model_formula = 'sex ~ bill_depth_mm + body_mass_g + bill_depth_mm:body_mass_g'

#train the data using logisitic regression
inter_model = smf.logit(formula = model_formula, data = train_set).fit()
inter_model.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.659308
         Iterations 5
```

Out[11]:

Logit Regression Results

Dep. Variable:	sex	**No. Observations:**	300
Model:	Logit	**Df Residuals:**	296
Method:	MLE	**Df Model:**	3
Date:	Sat, 02 Mar 2024	**Pseudo R-squ.:**	0.04870
Time:	09:25:31	**Log-Likelihood:**	-197.79
converged:	True	**LL-Null:**	-207.92
Covariance Type:	nonrobust	**LLR p-value:**	0.0001506

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	-0.2151	0.369	-0.583	0.560	-0.938	0.508
bill_depth_mm	0.0280	0.011	2.470	0.014	0.006	0.050
body_mass_g	-0.0203	0.012	-1.664	0.096	-0.044	0.004
bill_depth_mm:body_mass_g	-6.366e-05	0.000	-0.247	0.805	-0.001	0.000

10-Fold cross-validation

The different models to test are:

1. full additive model
2. reduced additive model 1
3. reduced additive model 2
4. interaction model

In [12]:

```
#define the target variable
target = 'sex'

#define the model formula
model_formulas = ['sex ~ species + island + bill_length_mm + bill_depth_mm + flipper_length_mm + body_mass_g',
                  'sex ~ species + island + bill_depth_mm + body_mass_g',
                  'sex ~ bill_depth_mm + body_mass_g',
                  'sex ~ bill_depth_mm + body_mass_g + bill_depth_mm:body_mass_g']

#perform cross-validation
model_accuracy = {}
```

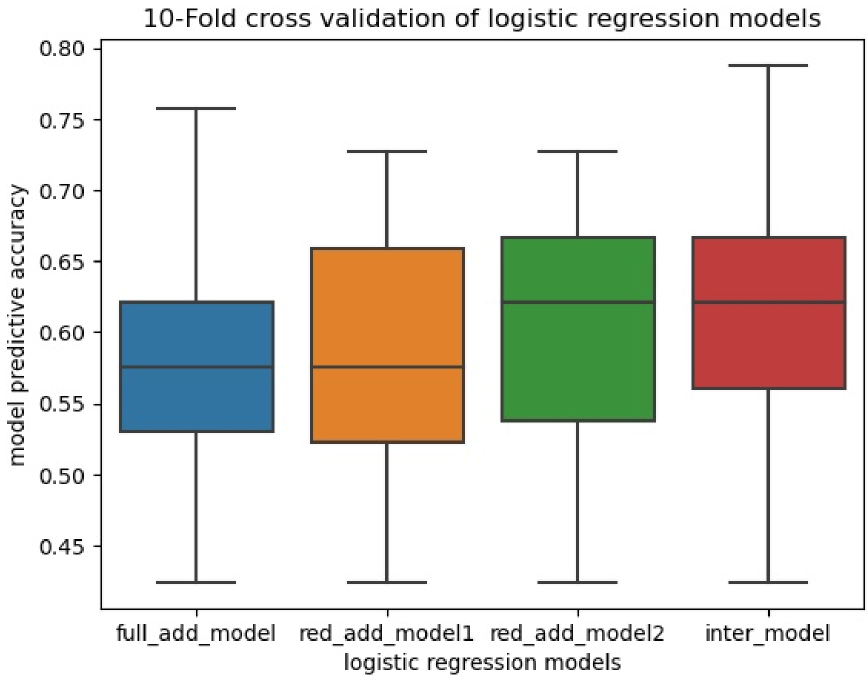
```python
for model_formula in model_formulas:
    fold_accuracy = []
    for i in range(len(train_test_sets)):
        #define train and test datasets
        test_set = train_test_sets[i][0]
        y_test = test_set[target]
        train_set = train_test_sets[i][1]

        #train the data using logistic regression
        model = smf.logit(formula = model_formula, data = train_set).fit(disp = 0)

        #make predictions using the model
        y_pred = model.predict(test_set)
        y_pred = (y_pred >= 0.5).astype(int)

        #test the accuracy of model predictions
        fold_accuracy.append(accuracy_score(y_test, y_pred))

    #store the accuracy results
    model_accuracy[model_formula] = fold_accuracy

#display model accuracy scores for each fold
model_accuracy = pd.DataFrame(model_accuracy)
model_accuracy.columns = ['full_add_model','red_add_model1','red_add_model2','inter_model']
model_accuracy
```

Out[12]:

	full_add_model	red_add_model1	red_add_model2	inter_model
0	0.515152	0.424242	0.424242	0.424242
1	0.575758	0.727273	0.696970	0.787879
2	0.727273	0.696970	0.727273	0.666667
3	0.575758	0.575758	0.606061	0.606061
4	0.575758	0.636364	0.666667	0.636364
5	0.636364	0.454545	0.515152	0.484848
6	0.484848	0.515152	0.515152	0.545455
7	0.757576	0.666667	0.666667	0.666667
8	0.575758	0.575758	0.606061	0.606061
9	0.424242	0.545455	0.636364	0.666667

In [13]:

```python
#display the accuracy scores for each model
sns.boxplot(model_accuracy)
plt.ylabel('model predictive accuracy')
plt.xlabel('logistic regression models')
plt.title('10-Fold cross validation of logistic regression models')
plt.show()
```



In [14]:

```python
#calculate the CV scores for each model
CV_results = model_accuracy.mean()
CV_results
```

Out[14]:
```
full_add_model     0.584848
red_add_model1     0.581818
red_add_model2     0.606061
inter_model        0.609091
dtype: float64
```

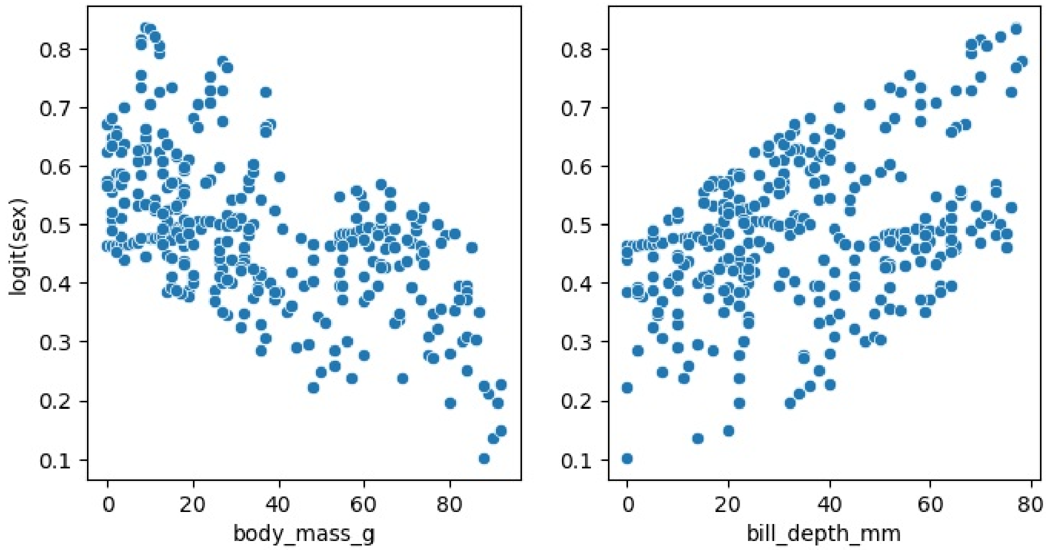
Based on the 10-fold cross validation accuracy scores, the *reduced additive model 2* and *interaction model* performed the best. Both models showed comparable performance but the simpler model is the *reduced additive model 2* and will therefore be used as the final model to classify penguin sex.

$$logit(sex) = -0.1462 + 0.0258 billdepth + 0.0229 bodymass + \epsilon$$

Checking final model assumptions

1. Binary response variable: Sex is either male or female.
2. Independence: Observations were measured independently for each individual penguin.
3. No multicollinearity among features: Collinear features were removed.
4. Linear relationship between features and logit of target variable: Shown below are the linear relationships for both feature variables.

In [15]:
```python
#calculate the log odds of the target variable
log_odds = red_add_model2.predict(df)

#define the subplot dimensions
fig, (ax1, ax2) = plt.subplots(nrows = 1, ncols = 2, figsize = (8,4))

#subplot 1
sns.scatterplot(x = 'body_mass_g', y = log_odds, data = df, ax = ax1)
ax1.set_ylabel('logit(sex)')

#subplot 2
sns.scatterplot(x = 'bill_depth_mm', y = log_odds, data = df, ax = ax2)

plt.show()
```



The final model satifies all assumptions of logistic regression.

Conclusion

The average cross-validation accuracy of the final model was 60.61%. More feature variables are needed to improve the predictive accuracy of this model to classify penguin sex.

Processing math: 100%