Machine Learning - Explain Models with SHAP

Classification

https://www.kaggle.com/parulpandey/palmer-archipelago-antarctica-penguin-data

In [ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import plotly.express as px
from sklearn.preprocessing import StandardScaler
from sklearn.tree import plot_tree
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
import shap
```

In [ ]:
```
penguins = pd.read_csv('penguins_size.csv')
penguins.head()
```

Out[ ]:

	species	island	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g	sex
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0	MALE
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0	FEMALE
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0	FEMALE
3	Adelie	Torgersen	NaN	NaN	NaN	NaN	NaN
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0	FEMALE

In [ ]:
```
penguins.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 344 entries, 0 to 343
Data columns (total 7 columns):
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   species            344 non-null    object 
 1   island             344 non-null    object 
 2   culmen_length_mm   342 non-null    float64
 3   culmen_depth_mm    342 non-null    float64
 4   flipper_length_mm  342 non-null    float64
 5   body_mass_g        342 non-null    float64
 6   sex                334 non-null    object 
dtypes: float64(4), object(3)
memory usage: 18.9+ KB
```

In [ ]:
```
penguins.describe(include='all')
```

Out[ ]:

	species	island	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g	sex
count	344	344	342.000000	342.000000	342.000000	342.000000	334
unique	3	3	NaN	NaN	NaN	NaN	3
top	Adelie	Biscoe	NaN	NaN	NaN	NaN	MALE
freq	152	168	NaN	NaN	NaN	NaN	168
mean	NaN	NaN	43.921930	17.151170	200.915205	4201.754386	NaN
std	NaN	NaN	5.459584	1.974793	14.061714	801.954536	NaN
min	NaN	NaN	32.100000	13.100000	172.000000	2700.000000	NaN
25%	NaN	NaN	39.225000	15.600000	190.000000	3550.000000	NaN
50%	NaN	NaN	44.450000	17.300000	197.000000	4050.000000	NaN
75%	NaN	NaN	48.500000	18.700000	213.000000	4750.000000	NaN
max	NaN	NaN	59.600000	21.500000	231.000000	6300.000000	NaN

In [ ]:
```
penguins.isna().sum()
```

Out[ ]:
```
species              0
island               0
culmen_length_mm     2
```

```
culmen_depth_mm       2
flipper_length_mm     2
body_mass_g           2
sex                  10
dtype: int64
```

In [ ]:
```
penguins = penguins.dropna()
penguins = penguins[penguins['sex'] != '.']
penguins = penguins.reset_index(drop=True)
penguins.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 333 entries, 0 to 332
Data columns (total 7 columns):
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   species            333 non-null    object 
 1   island             333 non-null    object 
 2   culmen_length_mm   333 non-null    float64
 3   culmen_depth_mm    333 non-null    float64
 4   flipper_length_mm  333 non-null    float64
 5   body_mass_g        333 non-null    float64
 6   sex                333 non-null    object 
dtypes: float64(4), object(3)
memory usage: 18.3+ KB
```

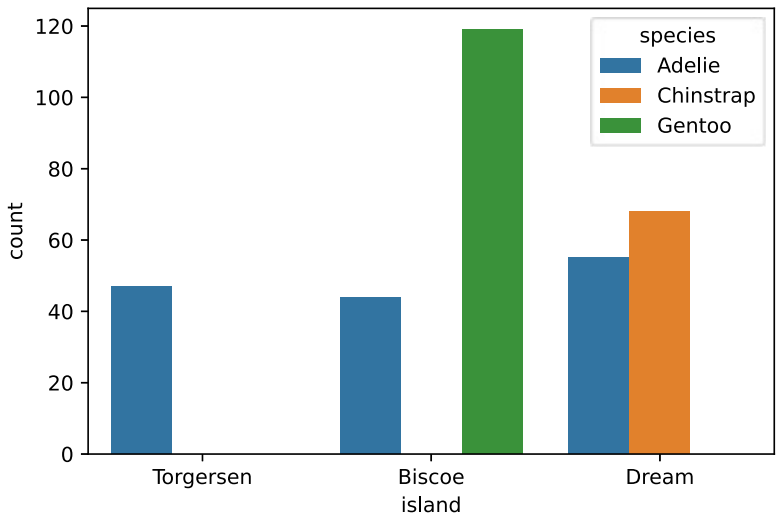
Exploratory Data Analysis

In [ ]:
```
val_count_cols = ['species', 'island', 'sex']
for col in val_count_cols:
    print(penguins[col].value_counts())
    print()
```

```
Adelie       146
Gentoo       119
Chinstrap     68
Name: species, dtype: int64

Biscoe       163
Dream        123
Torgersen     47
Name: island, dtype: int64

MALE      168
FEMALE    165
Name: sex, dtype: int64
```

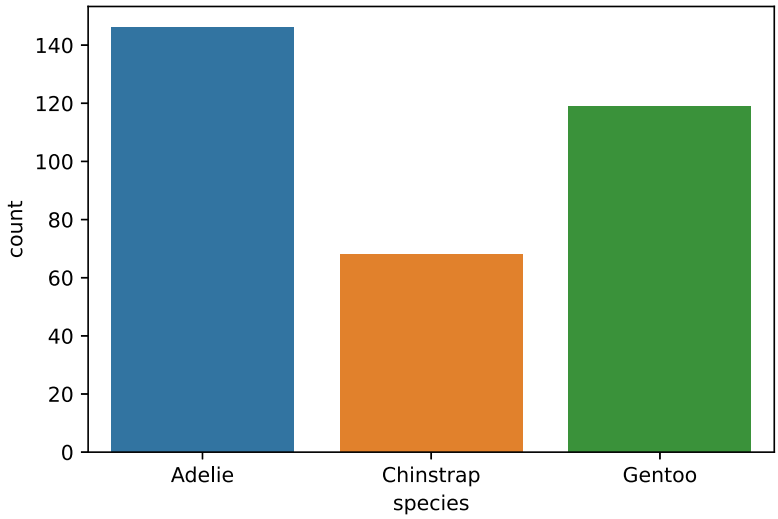
In [ ]:
```
sns.countplot(data=penguins, x='island', hue='species')
```

Out[ ]:
```
<AxesSubplot:xlabel='island', ylabel='count'>
```



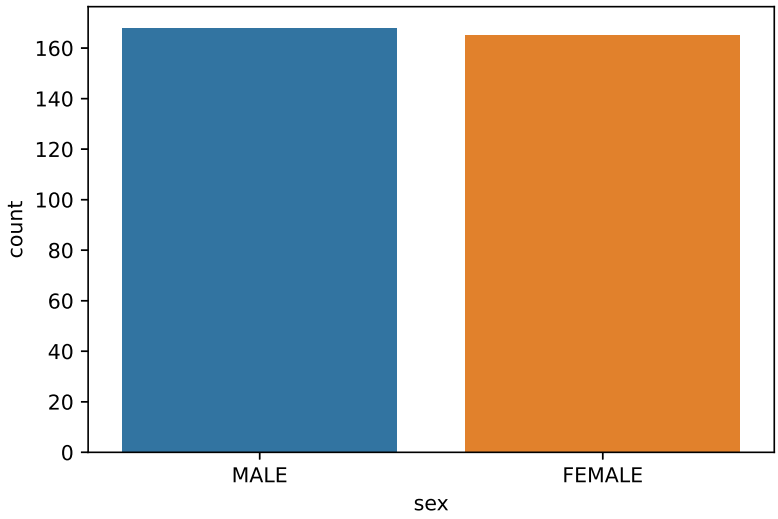
In [ ]:
```
sns.countplot(data=penguins, x='species')
```

Out[ ]: <AxesSubplot:xlabel='species', ylabel='count'>



In [ ]:
```
sns.countplot(data=penguins, x='sex')
```

Out[ ]: <AxesSubplot:xlabel='sex', ylabel='count'>



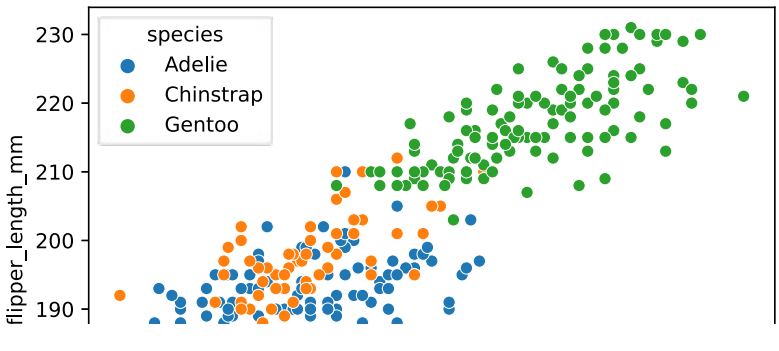
In [ ]:
```
penguins.corr()
```

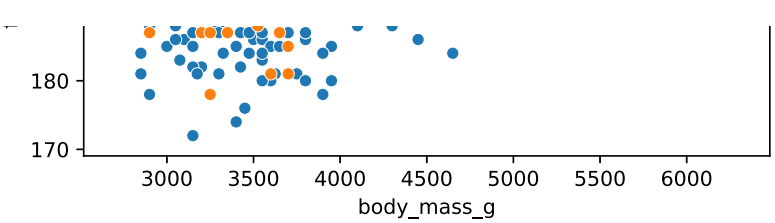
Out[ ]:

	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g
culmen_length_mm	1.000000	-0.228626	0.653096	0.589451
culmen_depth_mm	-0.228626	1.000000	-0.577792	-0.472016
flipper_length_mm	0.653096	-0.577792	1.000000	0.872979
body_mass_g	0.589451	-0.472016	0.872979	1.000000

In [ ]:
```
sns.scatterplot(data=penguins, x='body_mass_g', y='flipper_length_mm', hue='species')
```

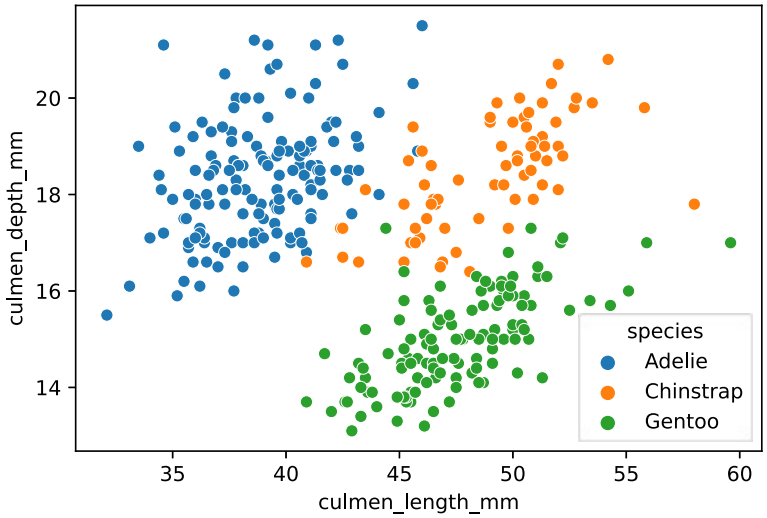
Out[ ]: <AxesSubplot:xlabel='body_mass_g', ylabel='flipper_length_mm'>





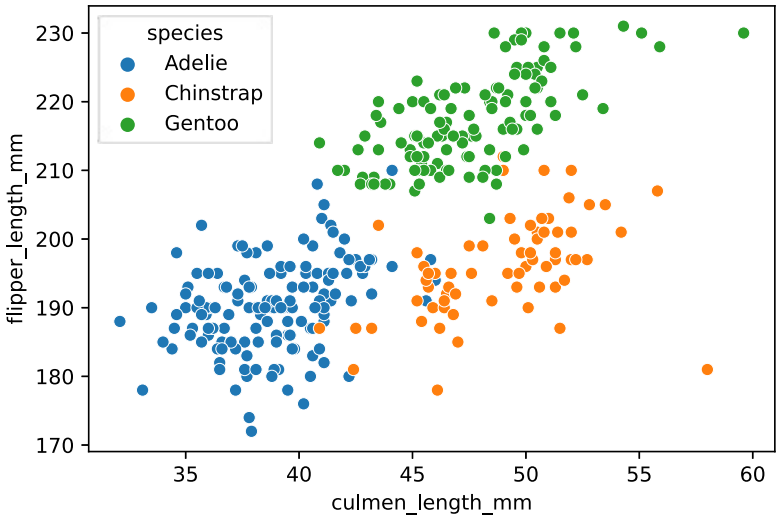
In [ ]:
```
sns.scatterplot(data=penguins, x='culmen_length_mm', y='culmen_depth_mm', hue='species')
```

Out[ ]: <AxesSubplot:xlabel='culmen_length_mm', ylabel='culmen_depth_mm'>



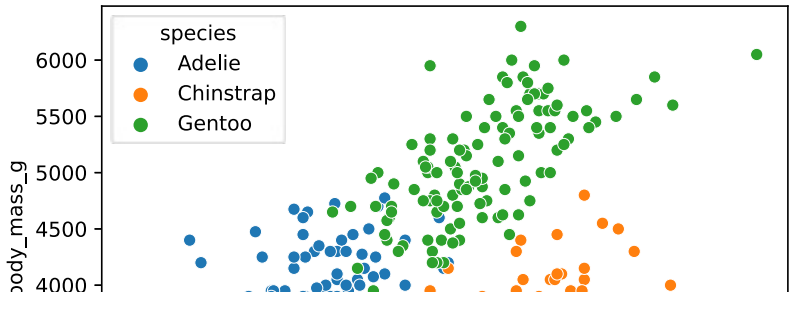
In [ ]:
```
sns.scatterplot(data=penguins, x='culmen_length_mm', y='flipper_length_mm', hue='species')
```

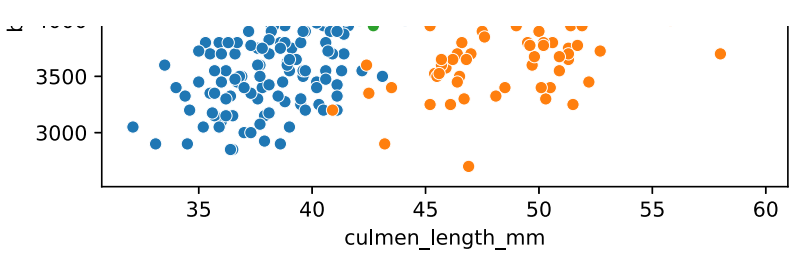
Out[ ]: <AxesSubplot:xlabel='culmen_length_mm', ylabel='flipper_length_mm'>



In [ ]:
```
sns.scatterplot(data=penguins, x='culmen_length_mm', y='body_mass_g', hue='species')
```

Out[ ]: <AxesSubplot:xlabel='culmen_length_mm', ylabel='body_mass_g'>





In [ ]:
```
px.scatter_3d(penguins, x='culmen_length_mm', y='culmen_depth_mm', z='flipper_length_mm', color='species', title=
```

In [ ]:
```
px.scatter_3d(penguins, x='culmen_length_mm', y='culmen_depth_mm', z='body_mass_g', color='species', title='Pengu
```

In [ ]:
```
px.scatter_3d(penguins, x='culmen_depth_mm', y='flipper_length_mm', z='body_mass_g', color='species', title='Peng
```

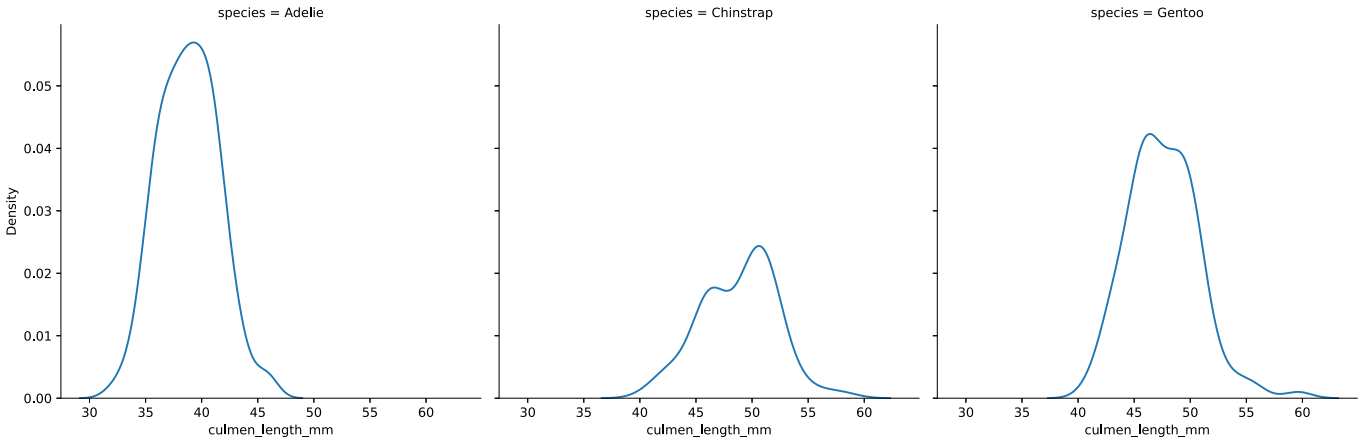
In [ ]:
```
px.scatter_3d(penguins, x='culmen_length_mm', y='flipper_length_mm', z='body_mass_g', color='species', title='Per
```

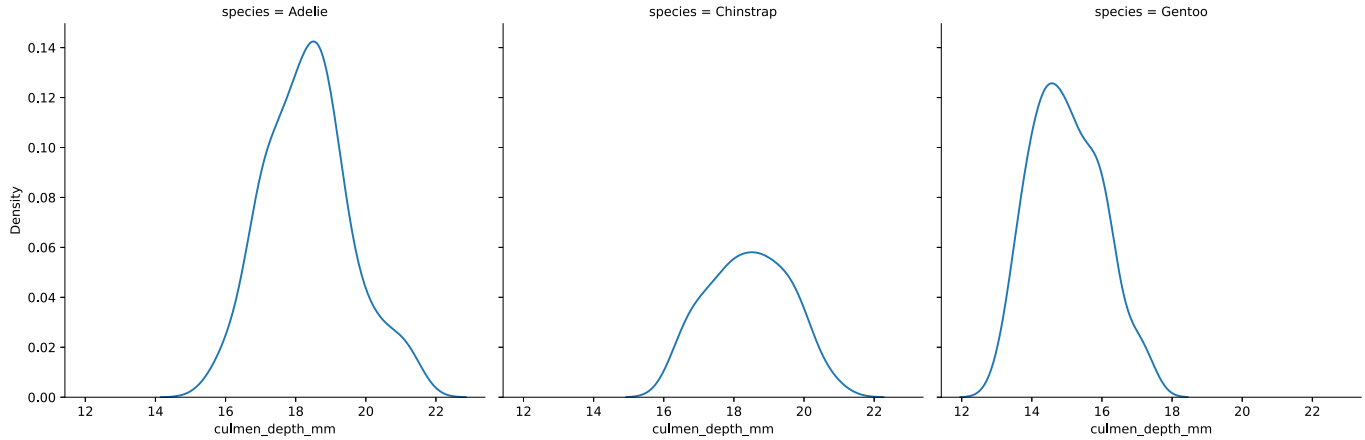
In [ ]:
```
penguins = penguins[['island', 'species', 'culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm', 'body_mass_
penguins.head()
```

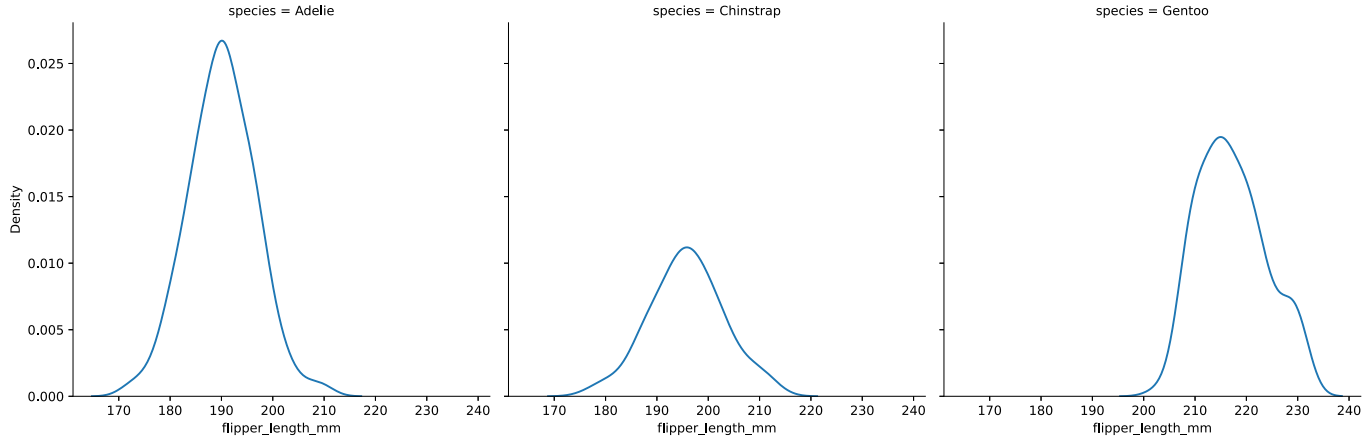
Out[ ]:

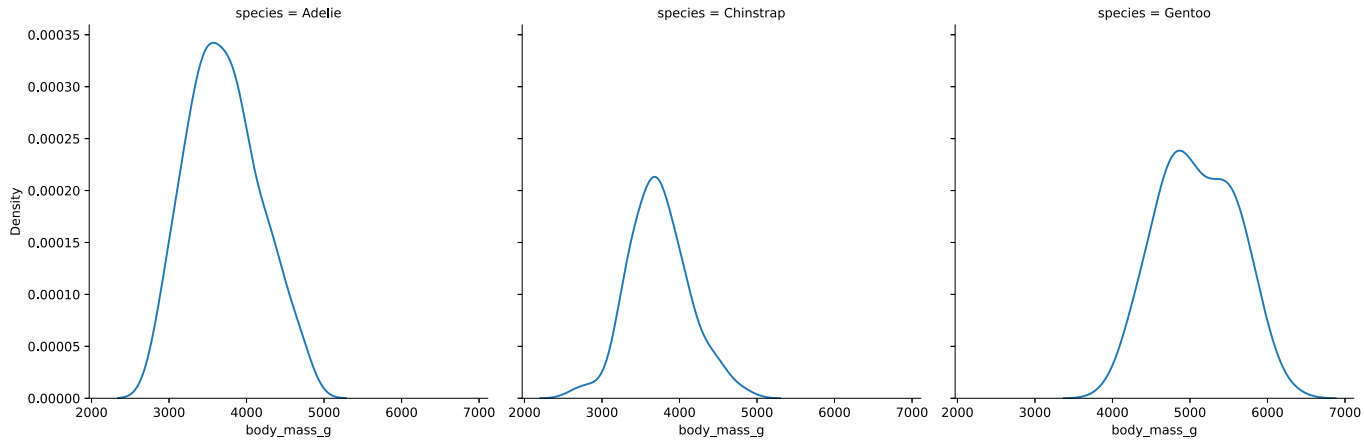
	island	species	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g	sex
0	Torgersen	Adelie	39.1	18.7	181.0	3750.0	MALE
1	Torgersen	Adelie	39.5	17.4	186.0	3800.0	FEMALE
2	Torgersen	Adelie	40.3	18.0	195.0	3250.0	FEMALE
3	Torgersen	Adelie	36.7	19.3	193.0	3450.0	FEMALE
4	Torgersen	Adelie	39.3	20.6	190.0	3650.0	MALE

In [ ]:
```
# plot distributions of numerical columns by species

plot_cols = ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm', 'body_mass_g']

for col in plot_cols:
    sns.displot(data=penguins, x=col, col='species', kind='kde')
```









In [ ]:
```
# statistics for each species
```

```
penguins.groupby('species').agg({'culmen_length_mm': ['count', 'min', 'max', 'mean', 'median'], 'culmen_depth_mm'
```

Out[ ]:

	culmen_length_mm					culmen_depth_mm					flipper_length_mm						
	count	min	max	mean	median	count	min	max	mean	median	count	min	max	mean	median	count	min
species																	
Adelie	146	32.1	46.0	38.823973	38.85	146	15.5	21.5	18.347260	18.40	146	172.0	210.0	190.102740	190.0	146	2850.0
Chinstrap	68	40.9	58.0	48.833824	49.55	68	16.4	20.8	18.420588	18.45	68	178.0	212.0	195.823529	196.0	68	2700.0
Gentoo	119	40.9	59.6	47.568067	47.40	119	13.1	17.3	14.996639	15.00	119	203.0	231.0	217.235294	216.0	119	3950.0

In [ ]:
```
# one hot encoding for categoricals

penguins = pd.get_dummies(penguins)
penguins.head()
```

Out[ ]:

	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g	island_Biscoe	island_Dream	island_Torgersen	species_Adelie	sp
0	39.1	18.7	181.0	3750.0	0	0	1	1	
1	39.5	17.4	186.0	3800.0	0	0	1	1	
2	40.3	18.0	195.0	3250.0	0	0	1	1	
3	36.7	19.3	193.0	3450.0	0	0	1	1	
4	39.3	20.6	190.0	3650.0	0	0	1	1	

In [ ]:
```
# independent and target variables

X = penguins.drop(columns='body_mass_g')
y = penguins['body_mass_g']

print(X.shape, y.shape)
```

```
(333, 11) (333,)
```

Random Forest Regressor -> predict body mass

In [ ]:
```
# split dataset into train and test

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=7)
print(X_train.shape, y_train.shape, X_test.shape, y_test.shape)
```

```
(266, 11) (266,) (67, 11) (67,)
```

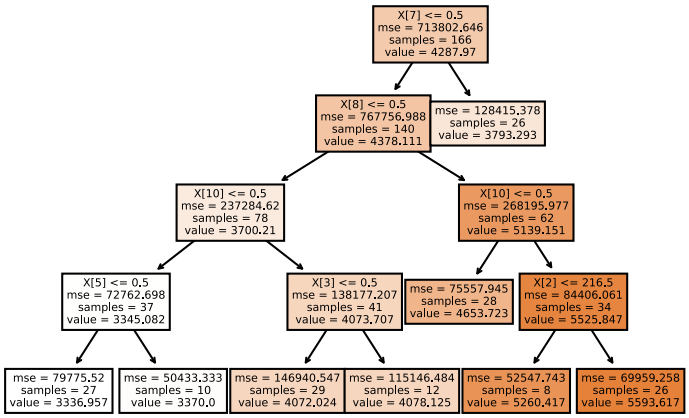
In [ ]:
```
# model

model = RandomForestRegressor(n_estimators=100, criterion='mse', max_depth=20, min_samples_split=30, max_features
model.fit(X_train, y_train)
```

Out[ ]:
```
RandomForestRegressor(max_depth=20, max_features=1, min_samples_split=30,
                      random_state=7)
```

In [ ]:
```
# plot for tree number 5 of the random forest model

from sklearn.tree import plot_tree

estimator = model.estimators_[5]

plot_tree(estimator, filled = True)
```

Out[ ]:
```
[Text(209.25000000000003, 195.696, 'X[7] <= 0.5\nmse = 713802.646\nsamples = 166\nvalue = 4287.97'),
 Text(181.35000000000002, 152.208, 'X[8] <= 0.5\nmse = 767756.988\nsamples = 140\nvalue = 4378.111'),
 Text(111.60000000000001, 108.72, 'X[10] <= 0.5\nmse = 237284.62\nsamples = 78\nvalue = 3700.21'),
 Text(55.800000000000004, 65.232, 'X[5] <= 0.5\nmse = 72762.698\nsamples = 37\nvalue = 3345.082'),
 Text(27.900000000000002, 21.744, 'mse = 79775.52\nsamples = 27\nvalue = 3336.957'),
 Text(83.7, 21.744, 'mse = 50433.333\nsamples = 10\nvalue = 3370.0'),
 Text(167.4, 65.232, 'X[3] <= 0.5\nmse = 138177.207\nsamples = 41\nvalue = 4073.707'),
 Text(139.5, 21.744, 'mse = 146940.547\nsamples = 29\nvalue = 4072.024'),
 Text(195.3, 21.744, 'mse = 115146.484\nsamples = 12\nvalue = 4078.125'),
 Text(251.10000000000002, 108.72, 'X[10] <= 0.5\nmse = 268195.977\nsamples = 62\nvalue = 5139.151'),
 Text(223.20000000000002, 65.232, 'mse = 75557.945\nsamples = 28\nvalue = 4653.723'),
```

```
Text(279.0, 65.232, 'X[2] <= 216.5\nmse = 84406.061\nsamples = 34\nvalue = 5525.847'),
Text(251.10000000000002, 21.744, 'mse = 52547.743\nsamples = 8\nvalue = 5260.417'),
Text(306.90000000000003, 21.744, 'mse = 69959.258\nsamples = 26\nvalue = 5593.617'),
Text(237.15, 152.208, 'mse = 128415.378\nsamples = 26\nvalue = 3793.293')]
```



In [ ]:
```
# predictions for train and test sets

y_pred_train = model.predict(X_train)
y_pred_test = model.predict(X_test)
```

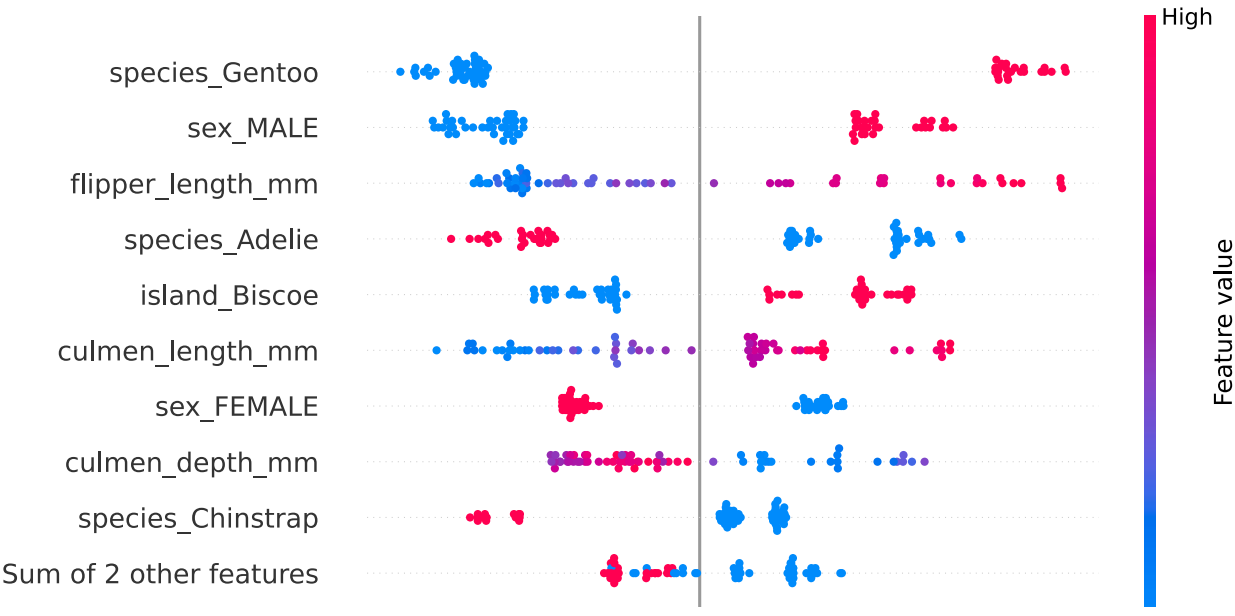
In [ ]:
```
# performance metrics for train and test sets

mae_train = mean_absolute_error(y_train, y_pred_train)
mse_train = mean_squared_error(y_train, y_pred_train)
r2_train = r2_score(y_train, y_pred_train)

mae_test = mean_absolute_error(y_test, y_pred_test)
mse_test = mean_squared_error(y_test, y_pred_test)
r2_test = r2_score(y_test, y_pred_test)

print(f'Train: MAE={mae_train} / MSE={mse_train} / R2: {r2_train}')
print(f'Test: MAE={mae_test} / MSE={mse_test} / R2: {r2_test}')
```

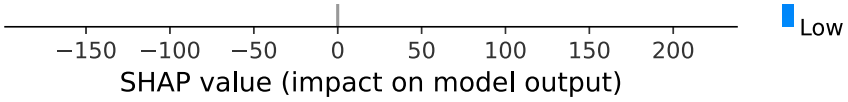
```
Train: MAE=227.24073991184062 / MSE=86006.69494581848 / R2: 0.869052917083086
Test: MAE=227.20652137525067 / MSE=78749.41899982275 / R2: 0.8669440122965669
```

Shap explainers

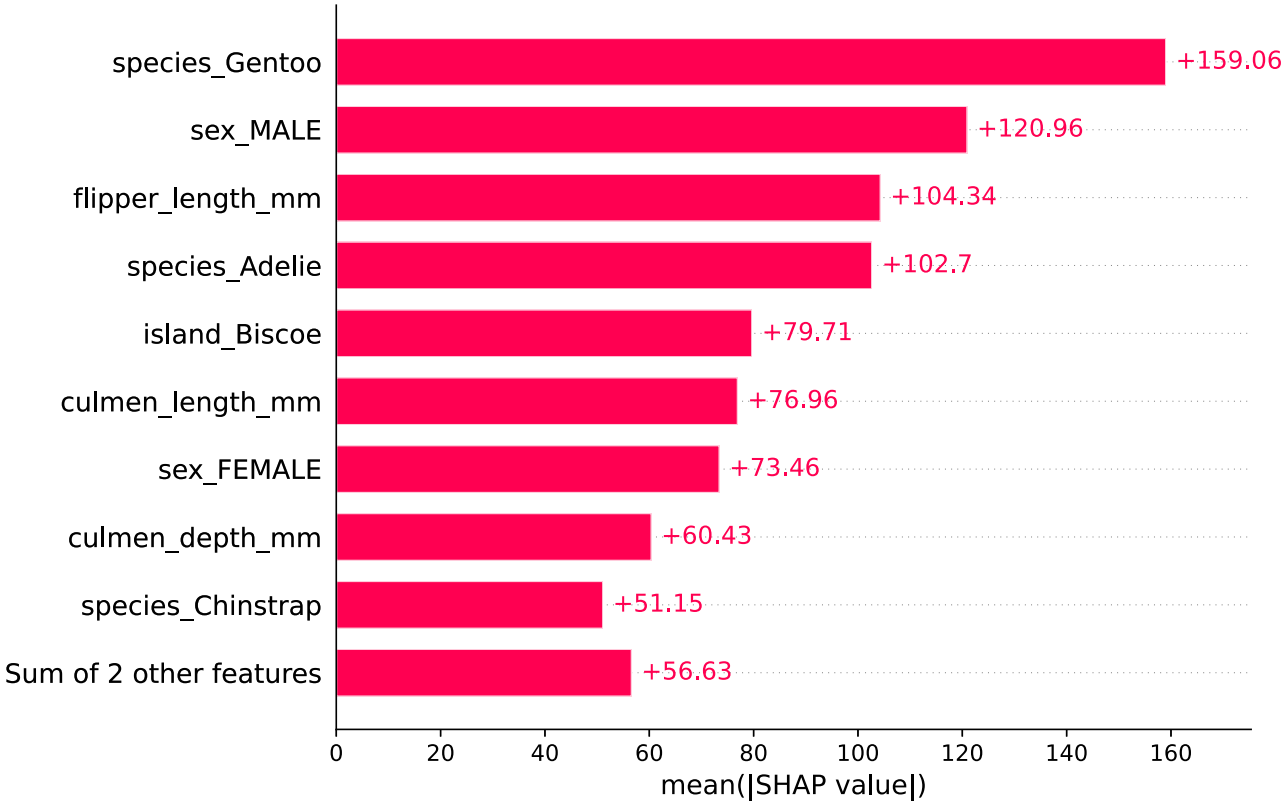
In [ ]:
```
explainer = shap.Explainer(model)
shap_values1 = explainer(X_test)
expected_value = explainer.expected_value

shap_values2 = shap_values = shap.TreeExplainer(model).shap_values(X_test)
```

In [ ]:
```
shap.plots.beeswarm(shap_values1)
```

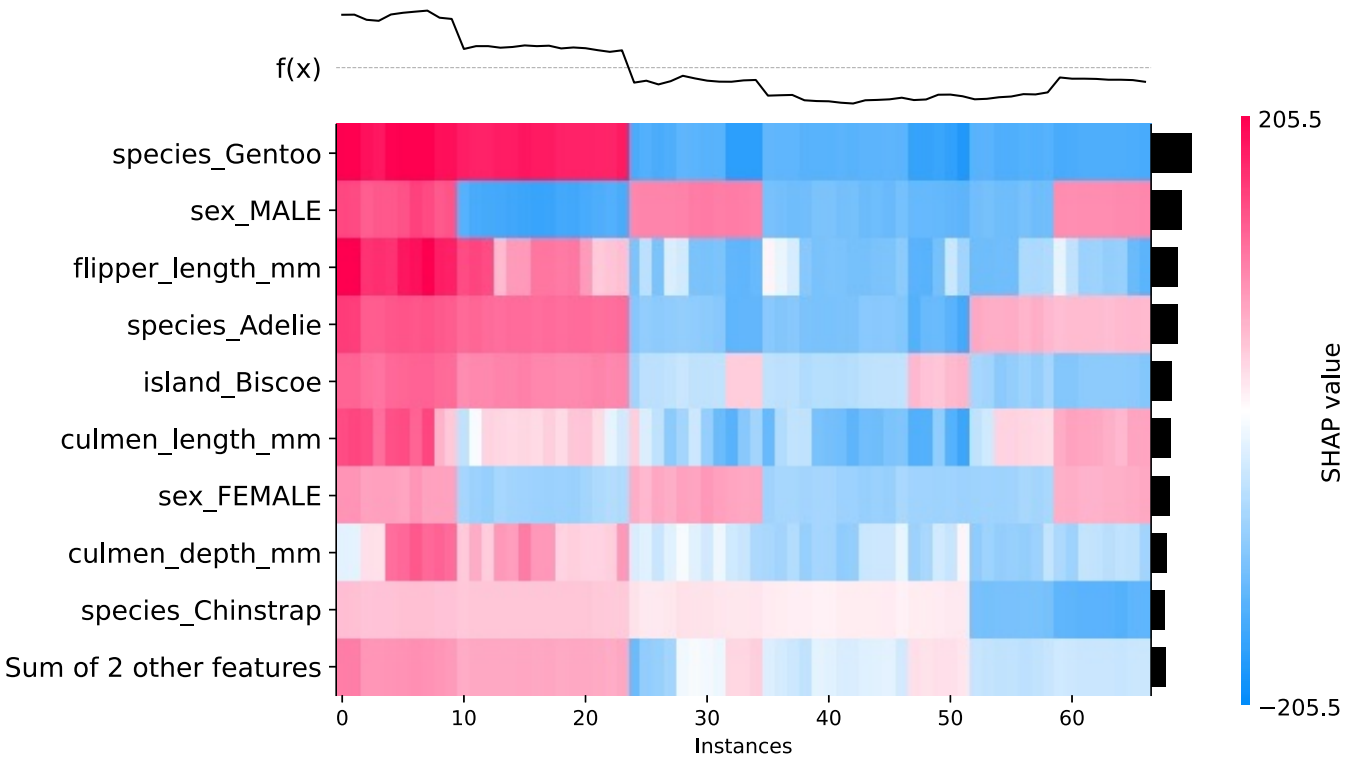




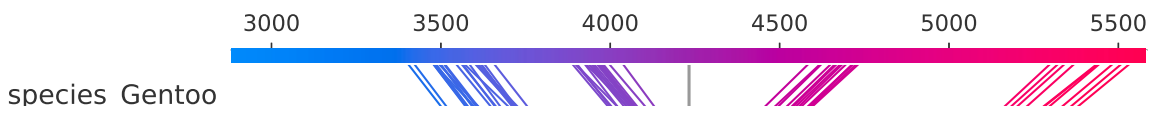
In [ ]:
```
shap.plots.bar(shap_values1)
```

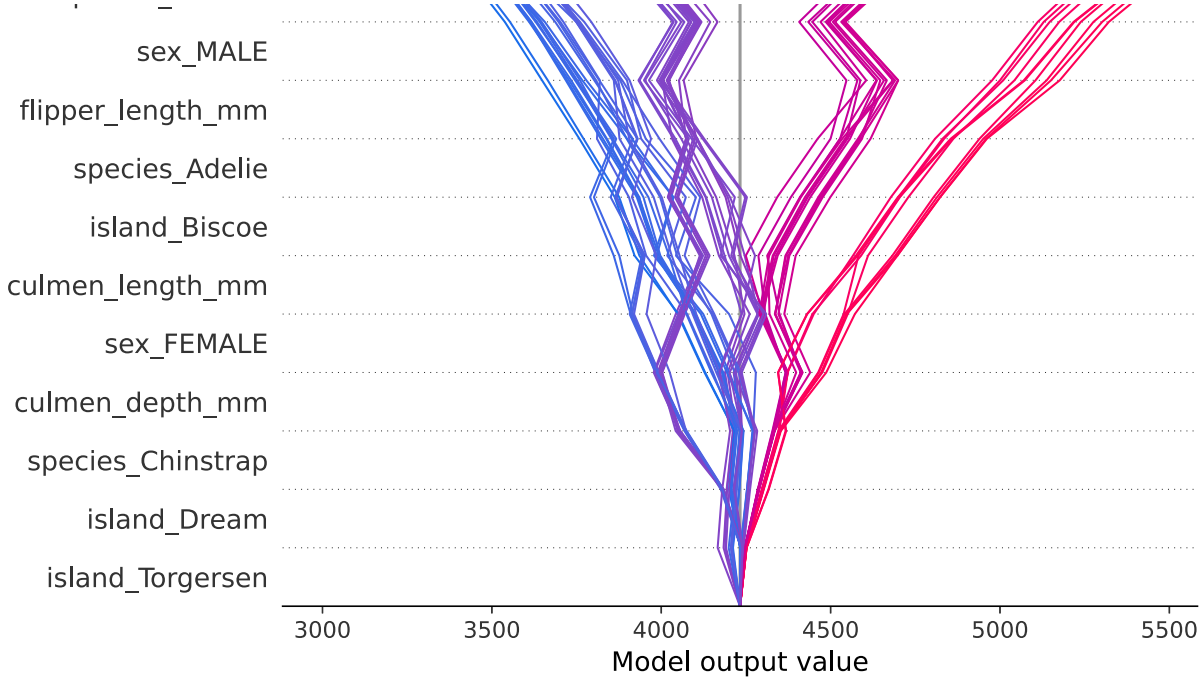


In [ ]:
```
shap.plots.heatmap(shap_values1)
```



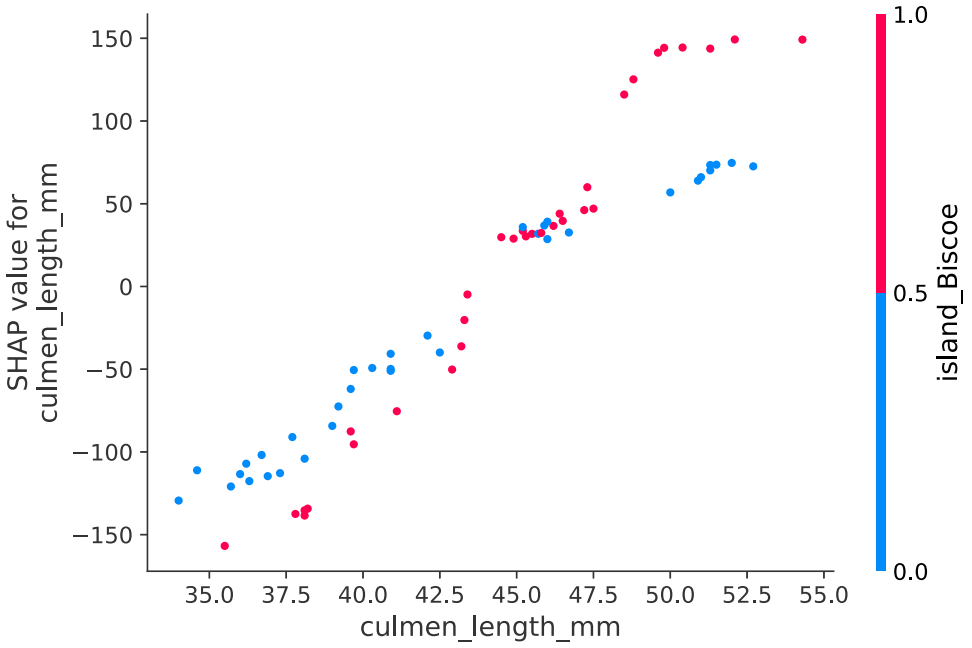
In [ ]:
```
shap.decision_plot(expected_value, shap_values2[:, :], X_test.iloc[:, :])
```





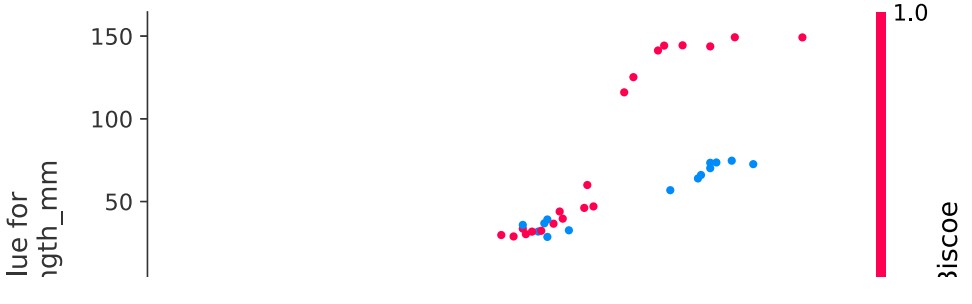
In [ ]:
```
shap.dependence_plot('culmen_length_mm', shap_values2, X_test)
```

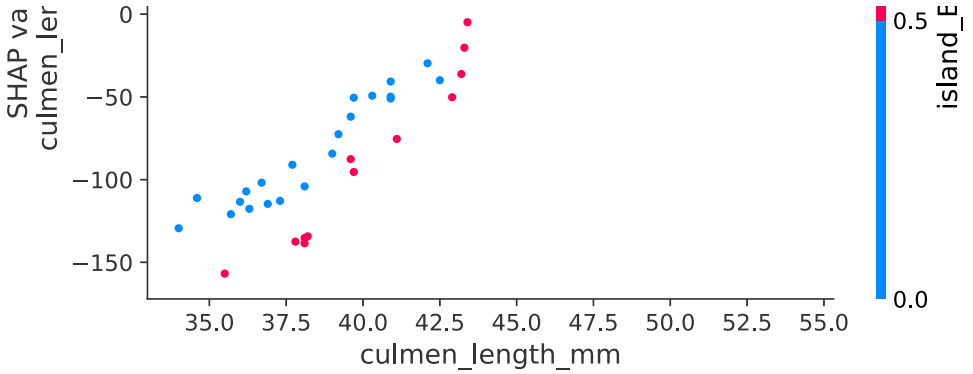
```
C:\Users\gulia\anaconda3\envs\tpot\lib\site-packages\shap\plots\_scatter.py:642: MatplotlibDeprecationWarning:

Passing parameters norm and vmin/vmax simultaneously is deprecated since 3.3 and will become an error two minor r
eleases later. Please pass vmin/vmax directly to the norm when creating it.
```



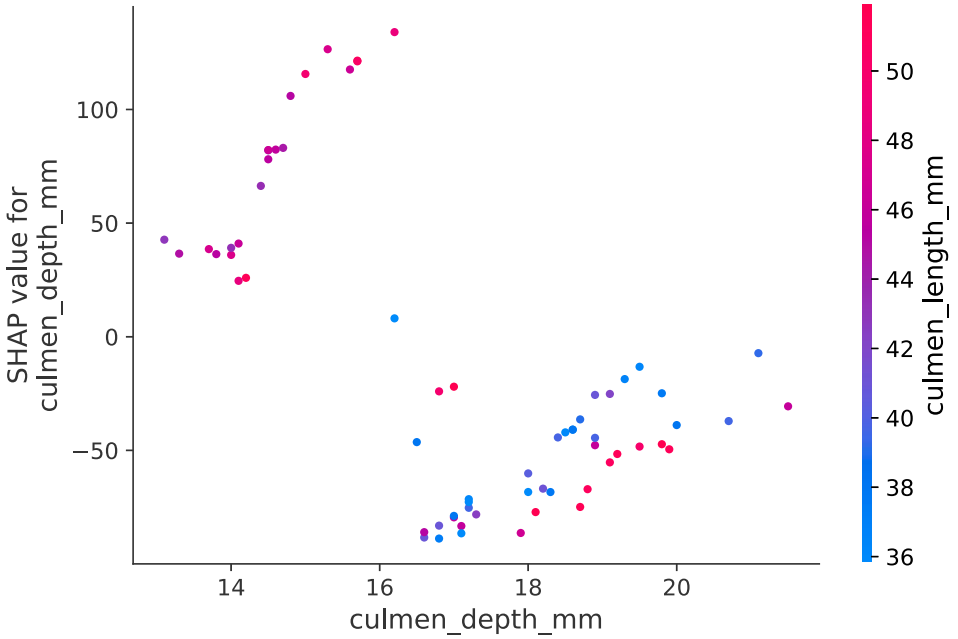
In [ ]:
```
shap.dependence_plot('culmen_length_mm', shap_values2, X_test)
```

```
C:\Users\gulia\anaconda3\envs\tpot\lib\site-packages\shap\plots\_scatter.py:642: MatplotlibDeprecationWarning:

Passing parameters norm and vmin/vmax simultaneously is deprecated since 3.3 and will become an error two minor r
eleases later. Please pass vmin/vmax directly to the norm when creating it.
```

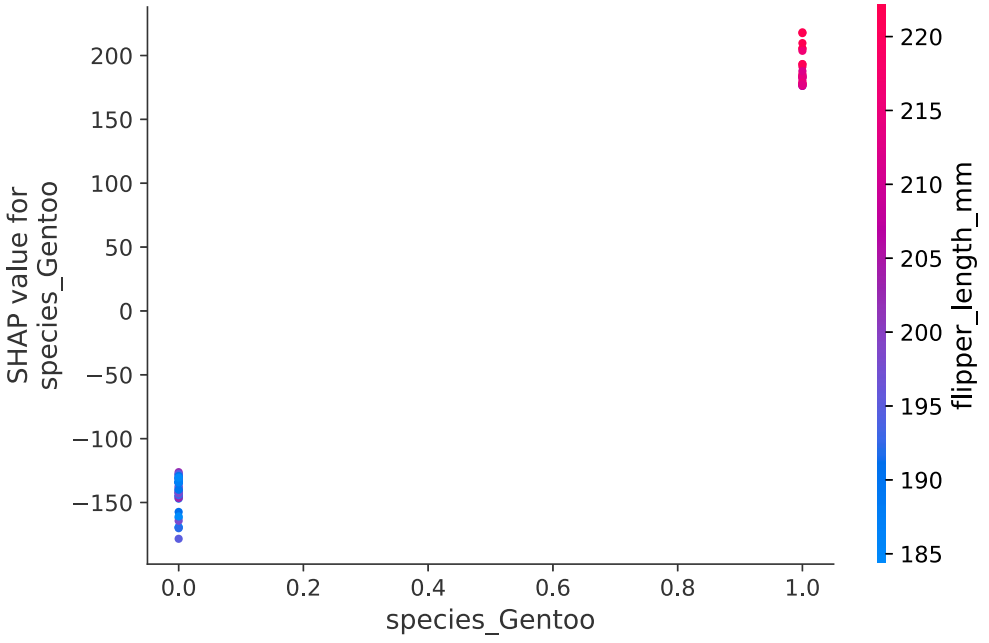




In [ ]:
```
shap.dependence_plot('culmen_depth_mm', shap_values2, X_test)
```



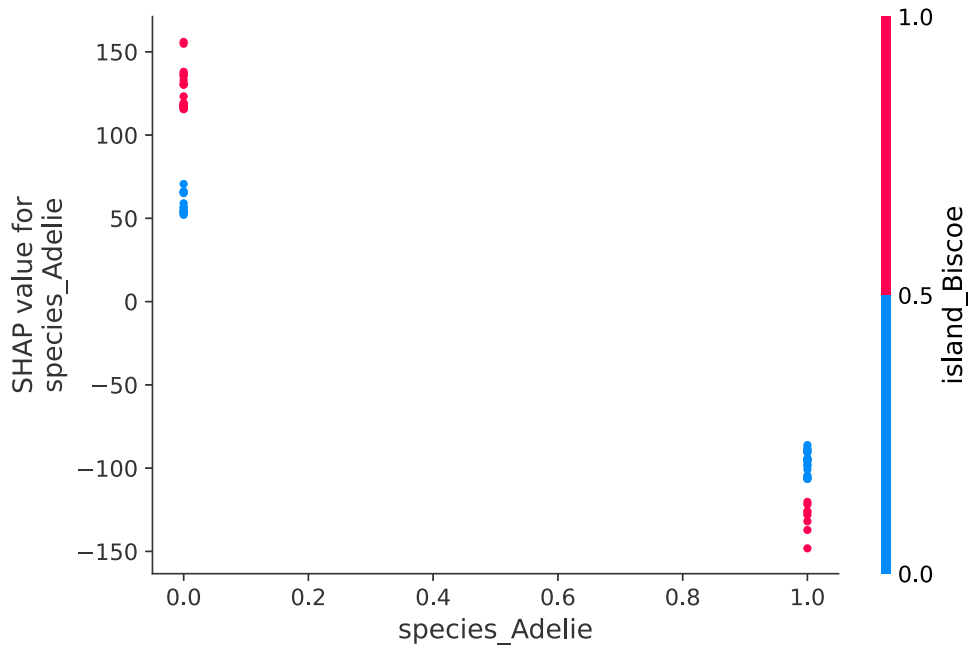
In [ ]:
```
shap.dependence_plot('species_Gentoo', shap_values2, X_test)
```



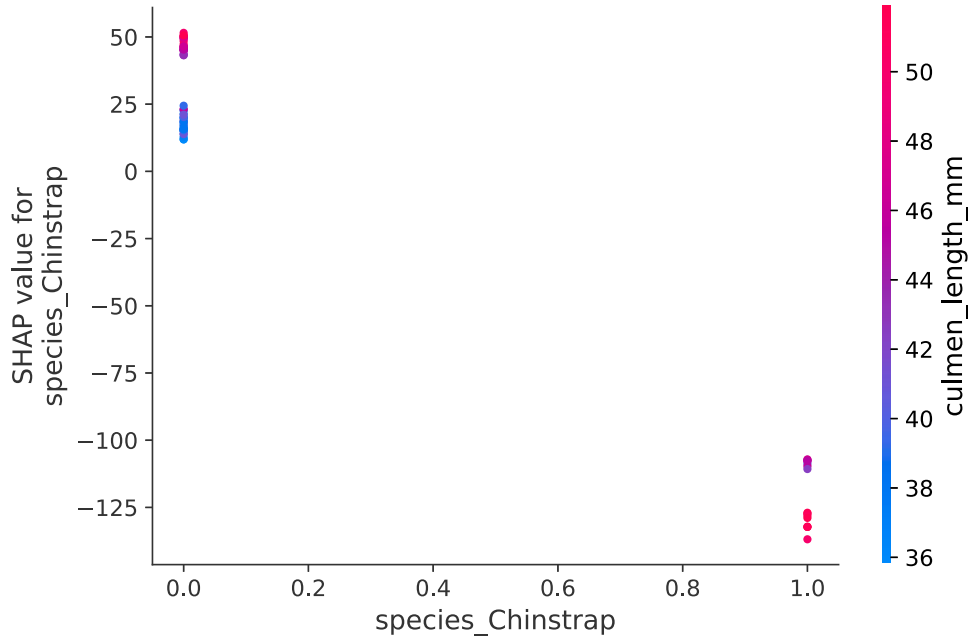
In [ ]:
```
shap.dependence_plot('species_Adelie', shap_values2, X_test)
```

```
C:\Users\gulia\anaconda3\envs\tpot\lib\site-packages\shap\plots\_scatter.py:642: MatplotlibDeprecationWarning:

Passing parameters norm and vmin/vmax simultaneously is deprecated since 3.3 and will become an error two minor r
```

```
eleases later. Please pass vmin/vmax directly to the norm when creating it.
```

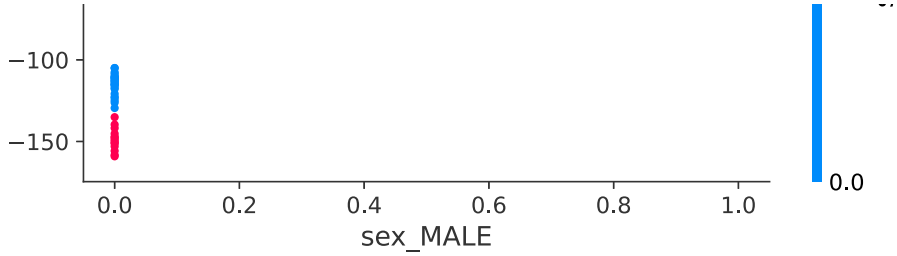


In [ ]:
```
shap.dependence_plot('species_Chinstrap', shap_values2, X_test)
```

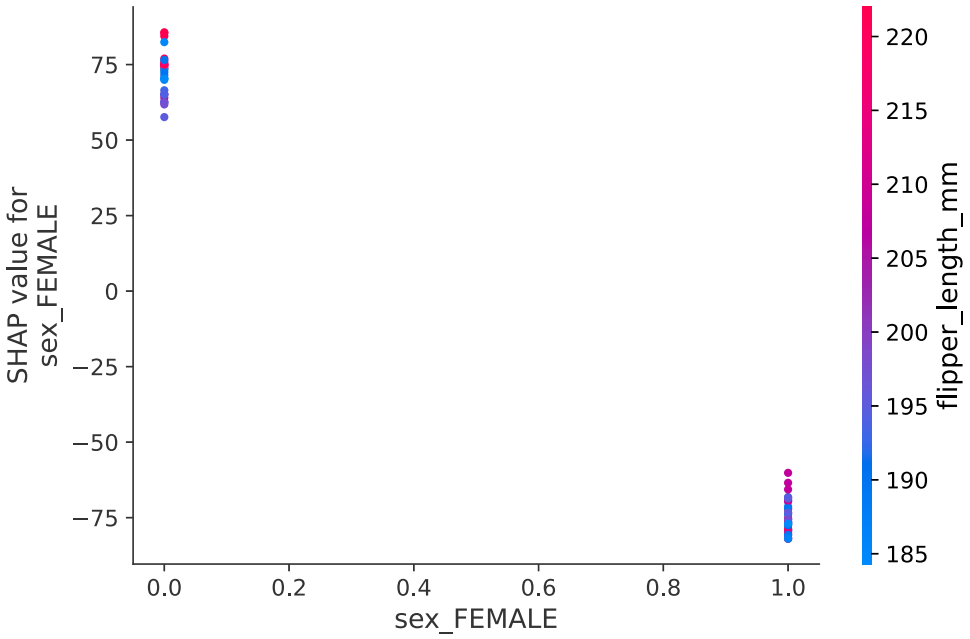


In [ ]:
```
shap.dependence_plot('sex_MALE', shap_values2, X_test)
```

```
C:\Users\gulia\anaconda3\envs\tpot\lib\site-packages\shap\plots\_scatter.py:642: MatplotlibDeprecationWarning:

Passing parameters norm and vmin/vmax simultaneously is deprecated since 3.3 and will become an error two minor r
eleases later. Please pass vmin/vmax directly to the norm when creating it.
```



In [ ]:
```
shap.dependence_plot('sex_FEMALE', shap_values2, X_test)
```



In [ ]:
```
shap.initjs()

def p(j):
    return(shap.force_plot(explainer.expected_value, shap_values2[j,:], X_test.iloc[j,:]))
```

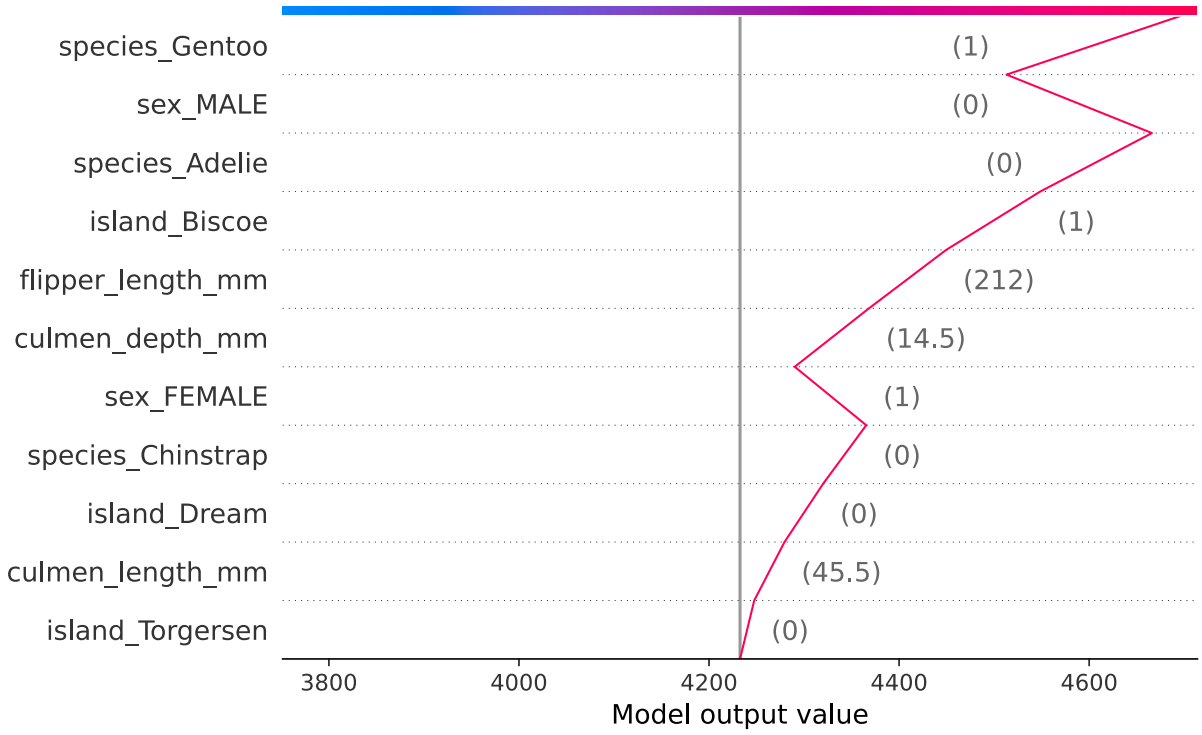
In [ ]:
```
shap.force_plot(expected_value, shap_values2, X_test.iloc[:, :])
```

Out[ ]:

In [ ]:
```
p(0)
```

Out[ ]:

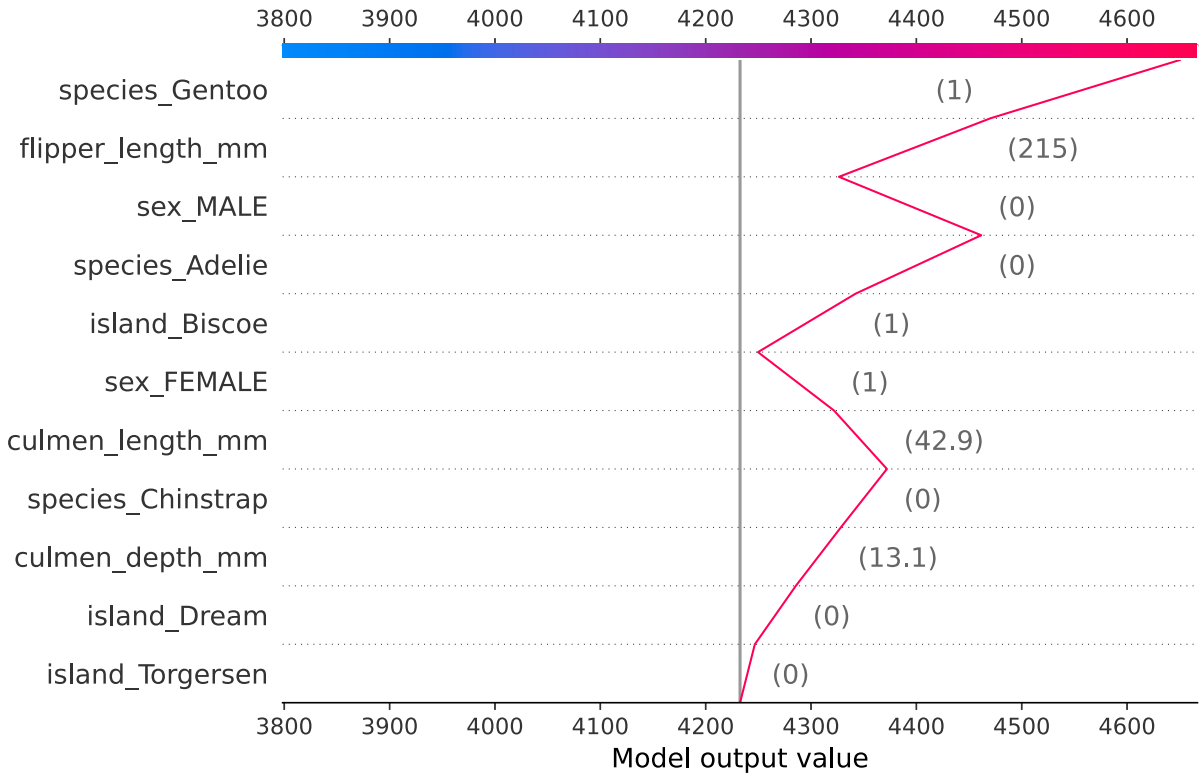
In [ ]:
```
shap.decision_plot(expected_value, shap_values2[0, :], X_test.iloc[0, :])
```



In [ ]:
```
p(33)
```

Out[ ]:

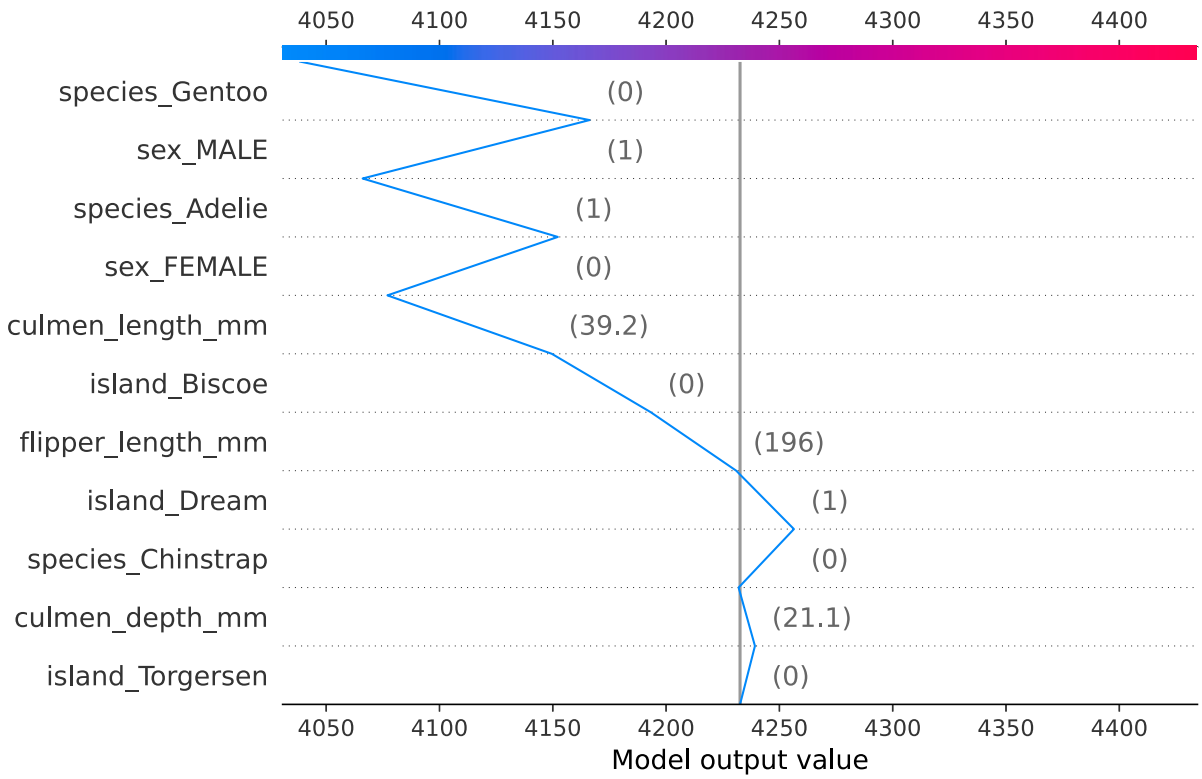
In [ ]:
```
shap.decision_plot(expected_value, shap_values2[33, :], X_test.iloc[33, :])
```



In [ ]:
```
p(7)
```

Out[ ]:

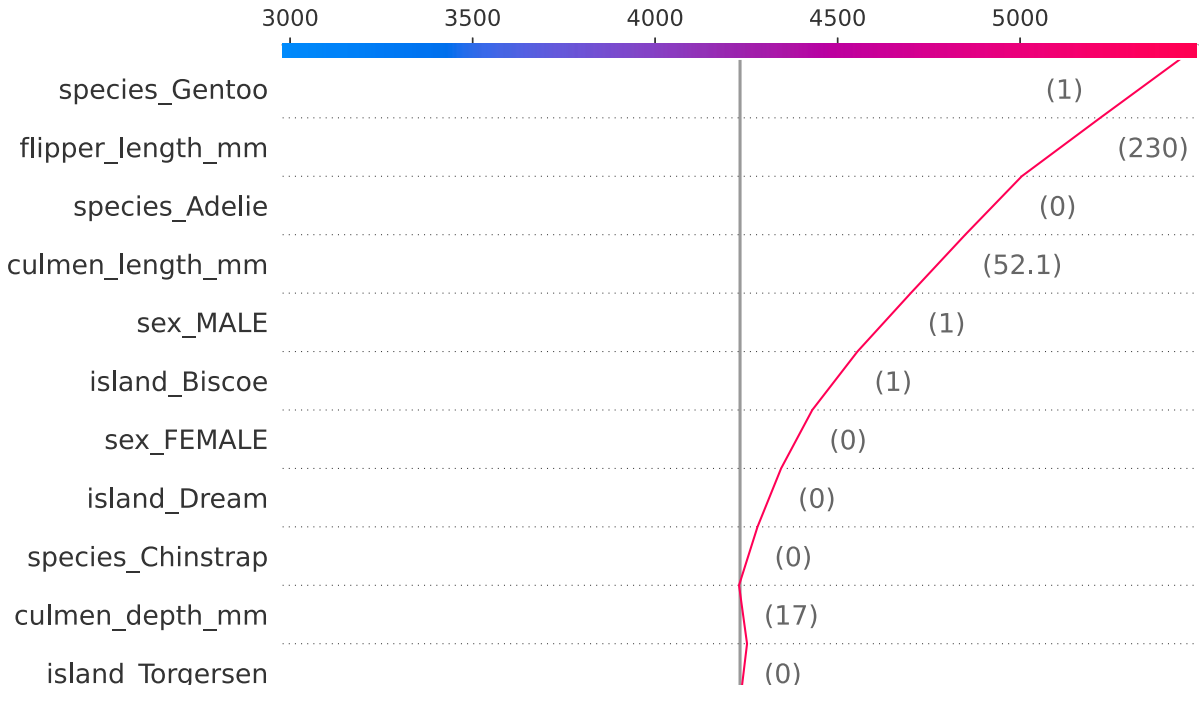
In [ ]:
```
shap.decision_plot(expected_value, shap_values2[7, :], X_test.iloc[7, :])
```

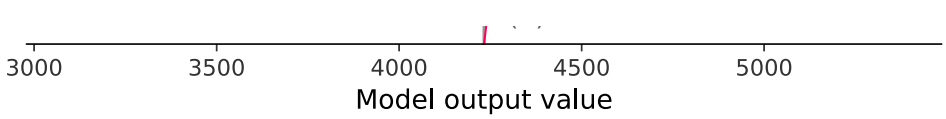


In [ ]:
```
p(27)
```

Out[ ]:

In [ ]:
```
shap.decision_plot(expected_value, shap_values2[27, :], X_test.iloc[27, :])
```





In [ ]: