GO DATA DRIVEN

Unpacking the Black Box

How to Interpret your Machine Learning Model

About us

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Organize

Data and AI Strategy Execution

Build

Data Platforms and AI Applications

Train

Data and AI Learning Journeys

Manage

Managed Data Platform and AI Services

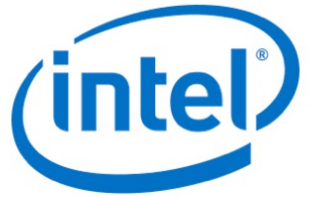
Democratize

Data Democratization

Solve

Turn-Key Cloud & Data Solutions

Trusted by global industry leaders



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GoDataDriven Academy

A variety of courses

- Data Science with Python (introductory & advanced)
- Deep Learning
- Data Visualisation & Storytelling
- Analytics Translation
- Time Series
- Machine Learning Explainability

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About you!

Join us at PollEverywhere

gdd.li/poll-amld

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Workshop outline

Topics are covered in the following way:

1. Experiment *first*
2. Explain *later*

Put it in practice:

- Hackathon
- Lightning talks!

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Workshop content

What we will cover:

- Intrinsicly explainable machine learning models
- Methods for model-agnostic interpretability
- Advantages and disadvantages of each method

What this workshop is **not** about:

- The theory behind every machine learning model (*algorithmic transparency)*
- Shapley values
- Neural networks

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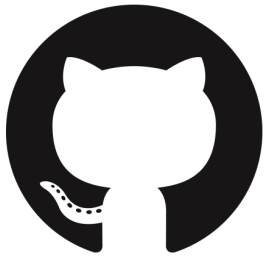
Material

Two ways to access the material:

1. **Binder**

   Does not require any installation

2. Download or clone the material from our **GitHub** repository



gdd.li/github

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Unpacking the black box

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History

- 1800s – Linear Regression
- 1960s – Decision Tree
- 2001 – Random Forests
- 2012 – Deep Learning
- 2016 – *Interpretable Machine Learning*

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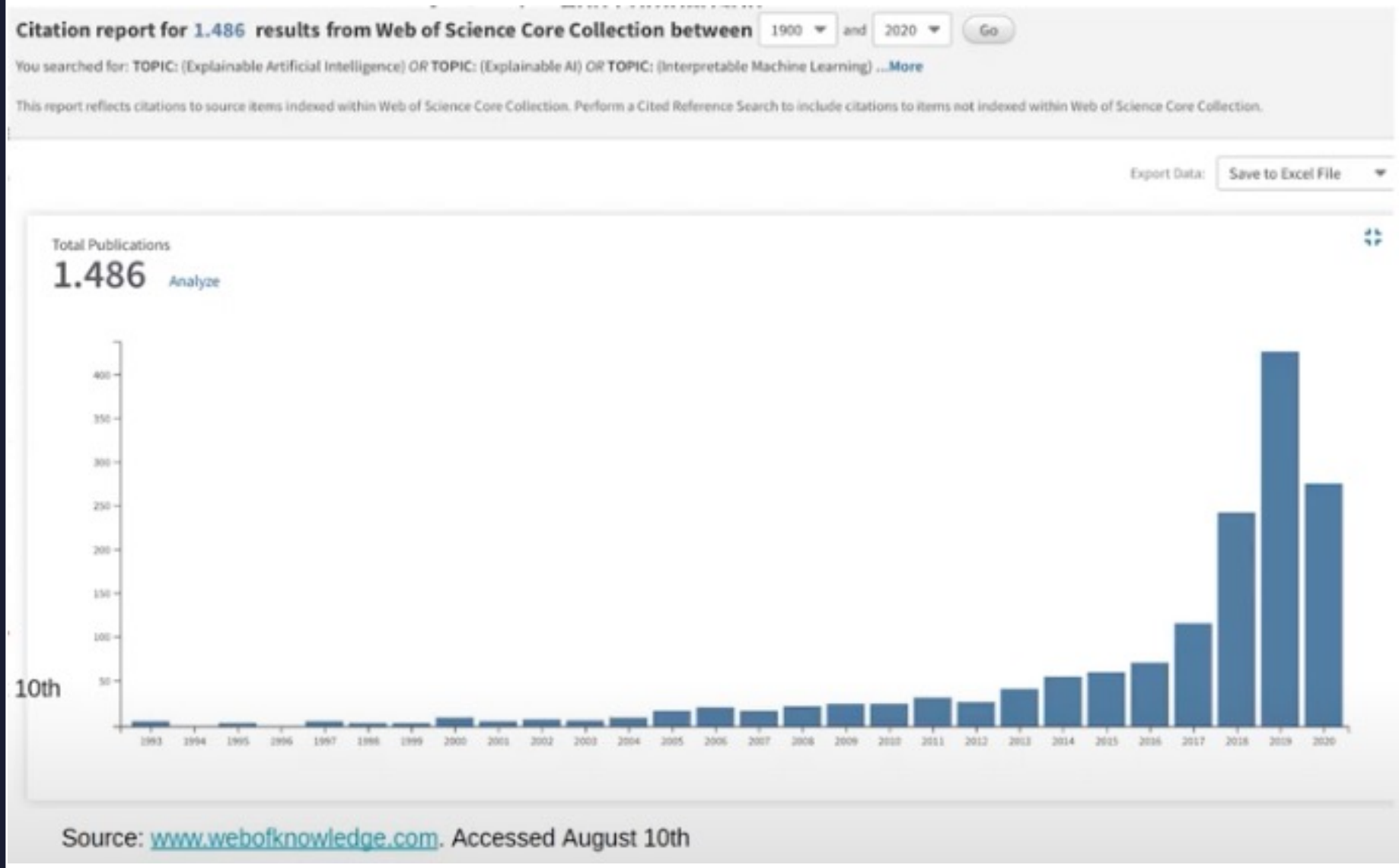

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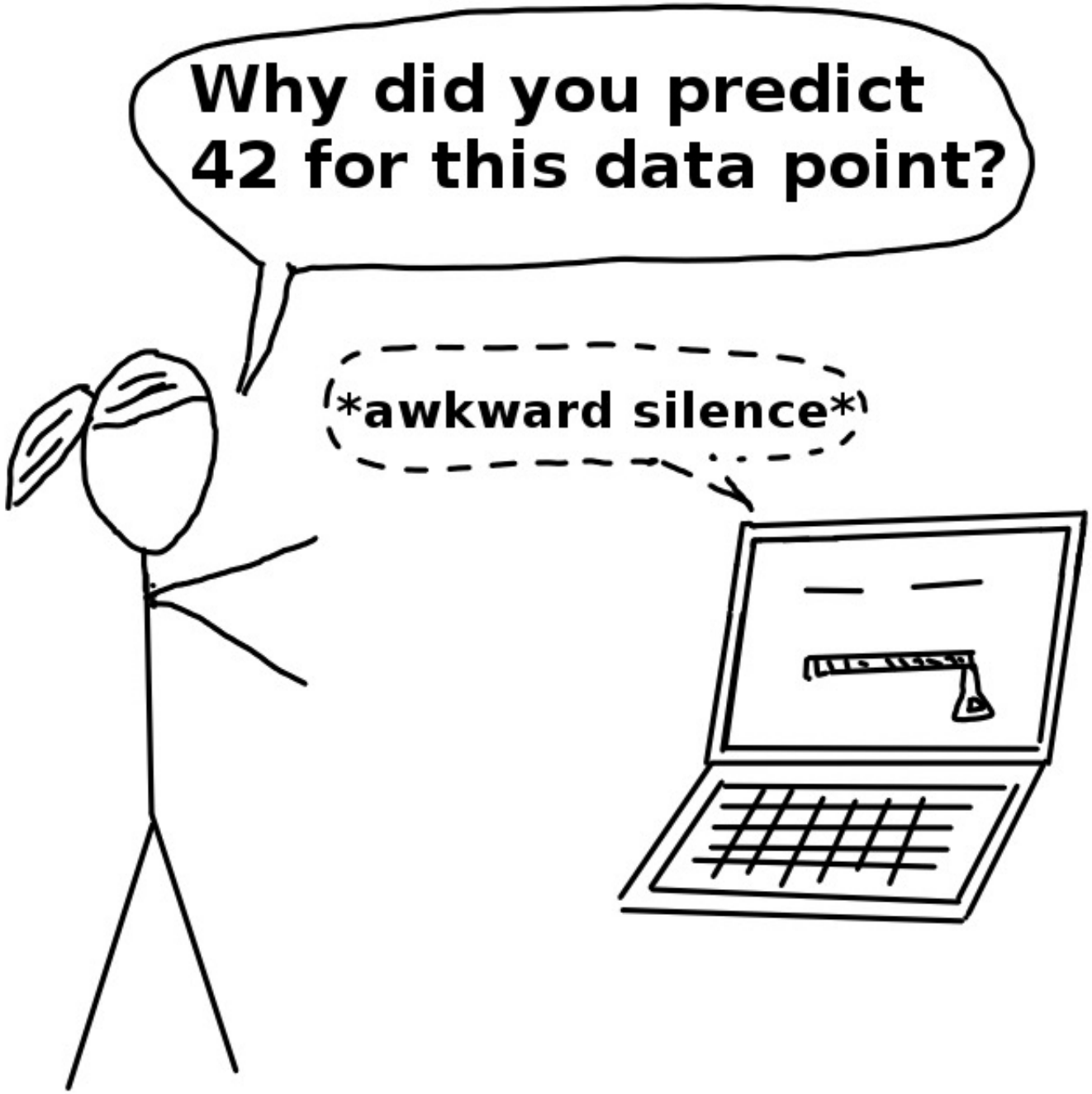
"Interpretability is the degree to which a human can understand the cause of a decision"

Source: Miller, Tim. "Explanation in artificial intelligence: Insights from the social sciences.

Why of Interpretability



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Why of Interpretability

- Engender trust

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Why of Interpretability

- Engender trust
- Right to explanation

Source: https://www.propublica.org/article/machine-bias-risk-assessments-in-criminal-sentencing

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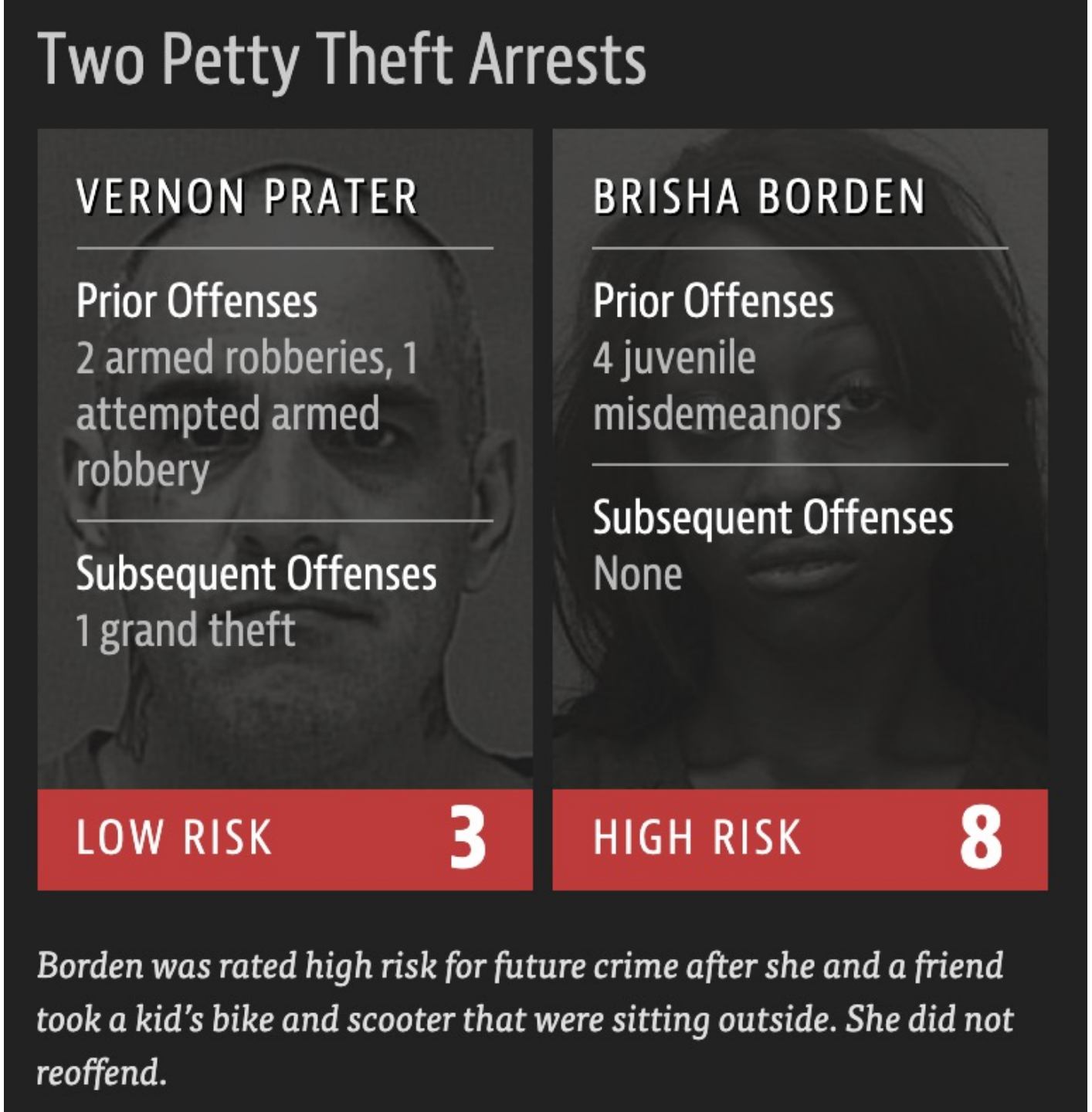

Why of Interpretability

- Engender trust
- Right to explanation
- **Debug models**

(a) Husky classified as wolf

(b) Explanation

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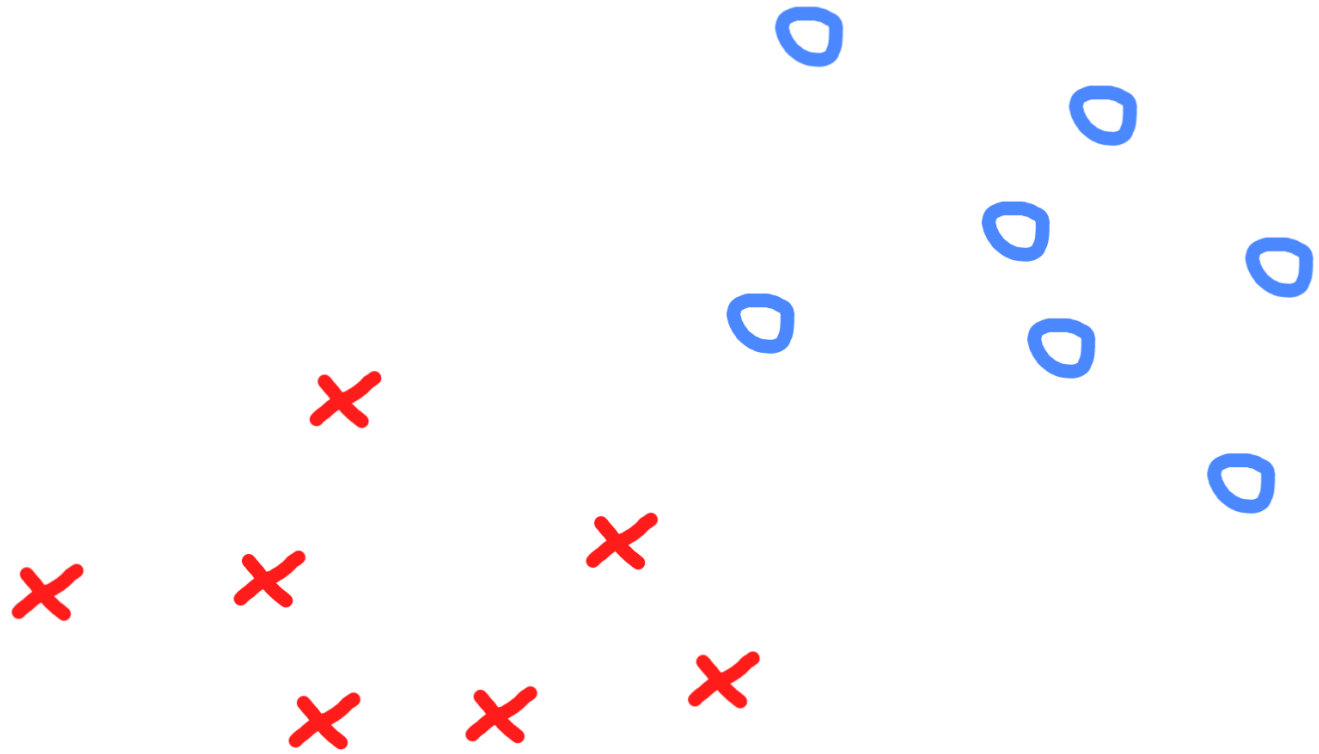
"Thing B is similar to thing A,
and thing A caused Y,
so I predict that B will cause Y!"

Example-based explanations

1. Some dataset with two classes



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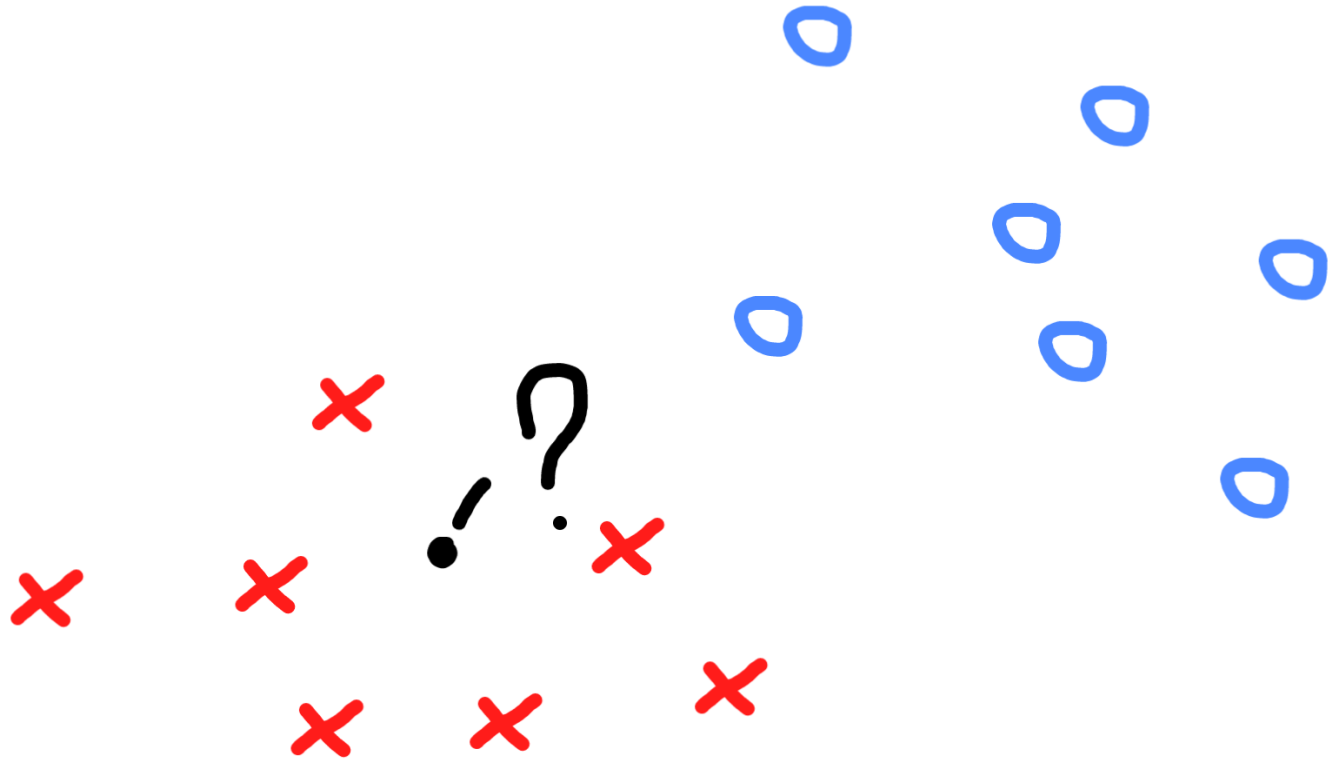
Example-based explanations

1. Some dataset with two classes
2. A new data point to classify



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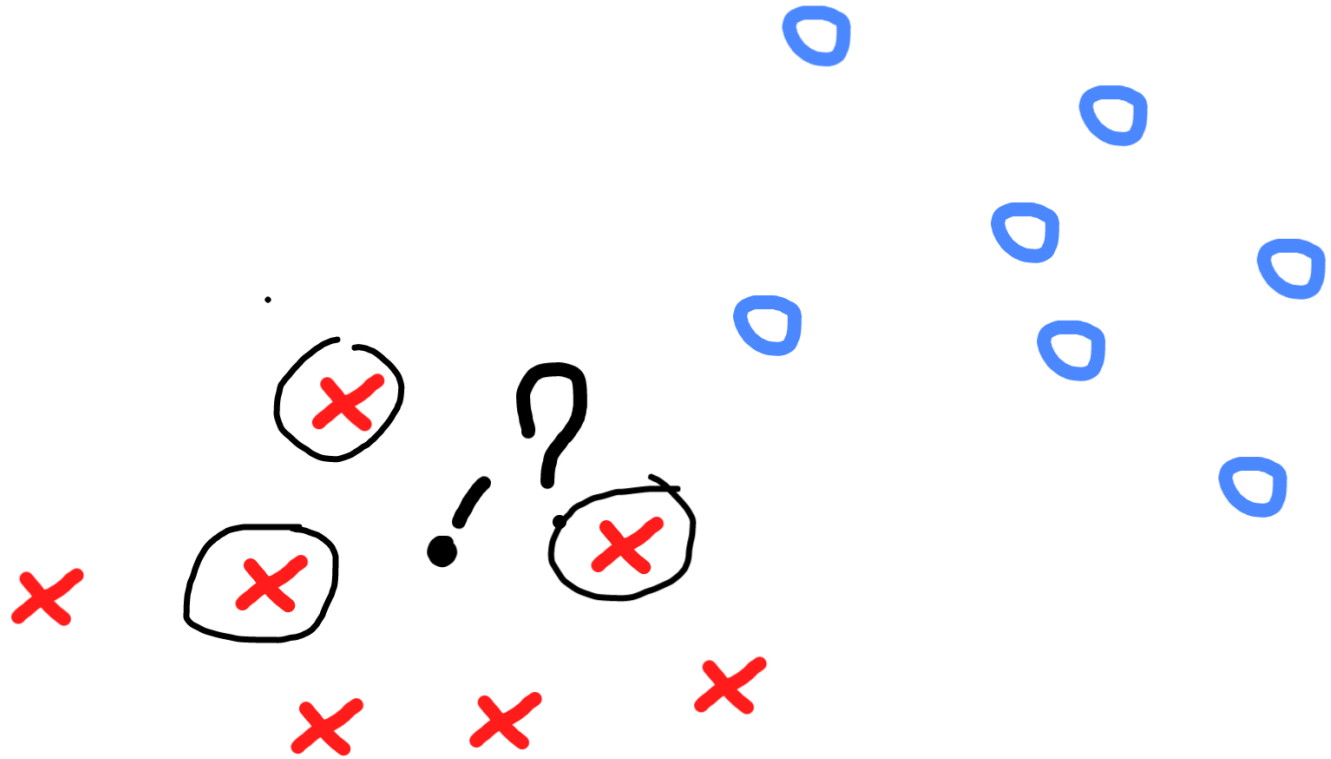
Example-based explanations

1. Some dataset with two classes
2. A new data point to classify
3. **An explanation based on nearby data points**



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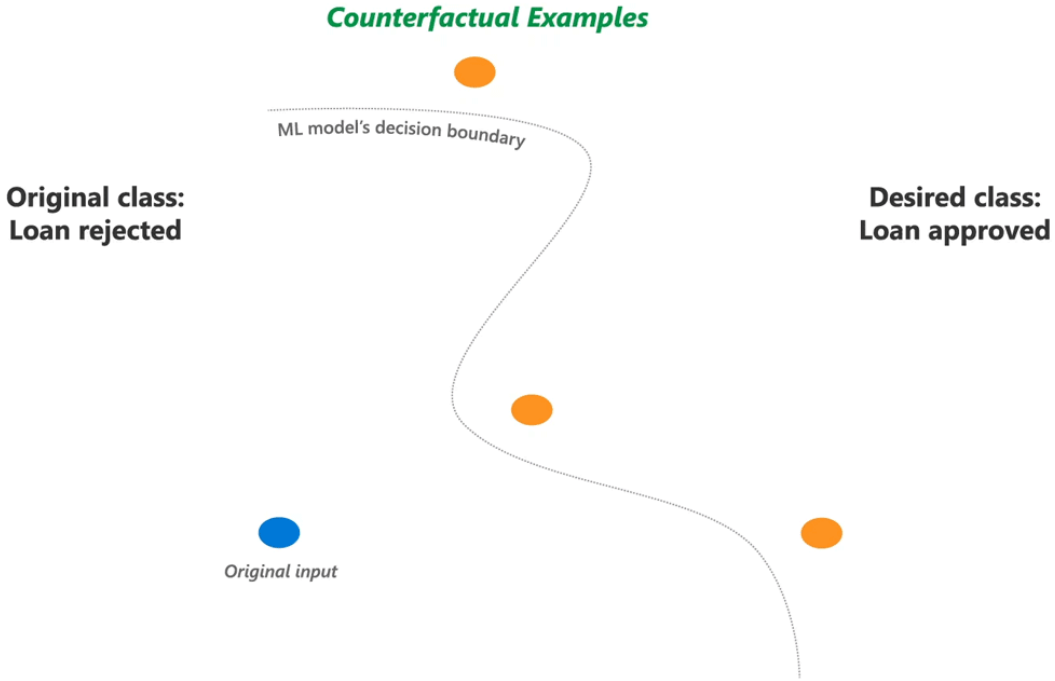
Example-based explanations

- Some models
- Counterfactual explanations
- Adversarial examples
- Prototypes & Criticisms
- Influential instances



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Jupyter Notebook 1

01_Introduction.ipynb

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The inherent interpretability of ML models

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Penguin 218

- Species: Chinstrap
- Flipper length: 210mm
- Body mass: 4100g

MISCLASSIFED AS GENTOO

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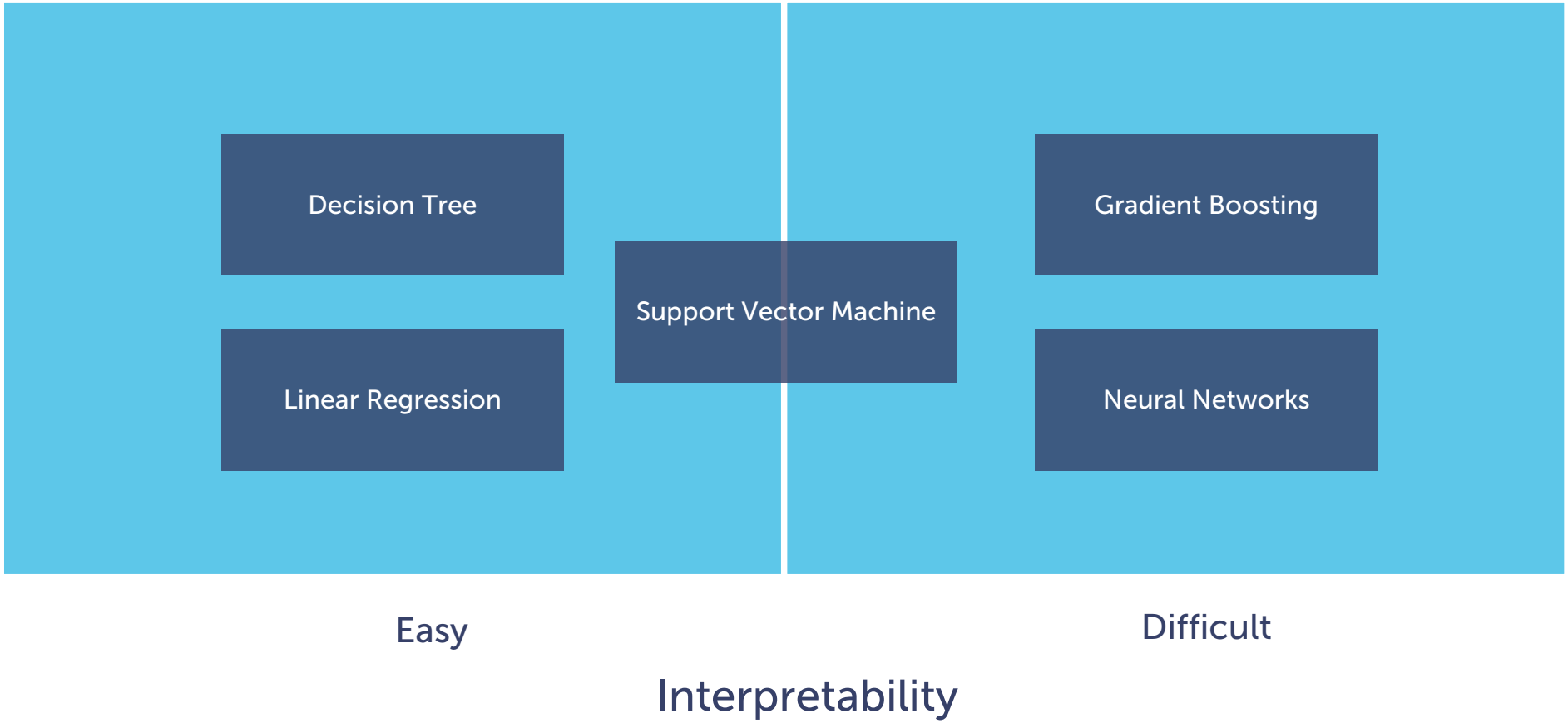
Inherent model interpretability



Decision Tree Classifer

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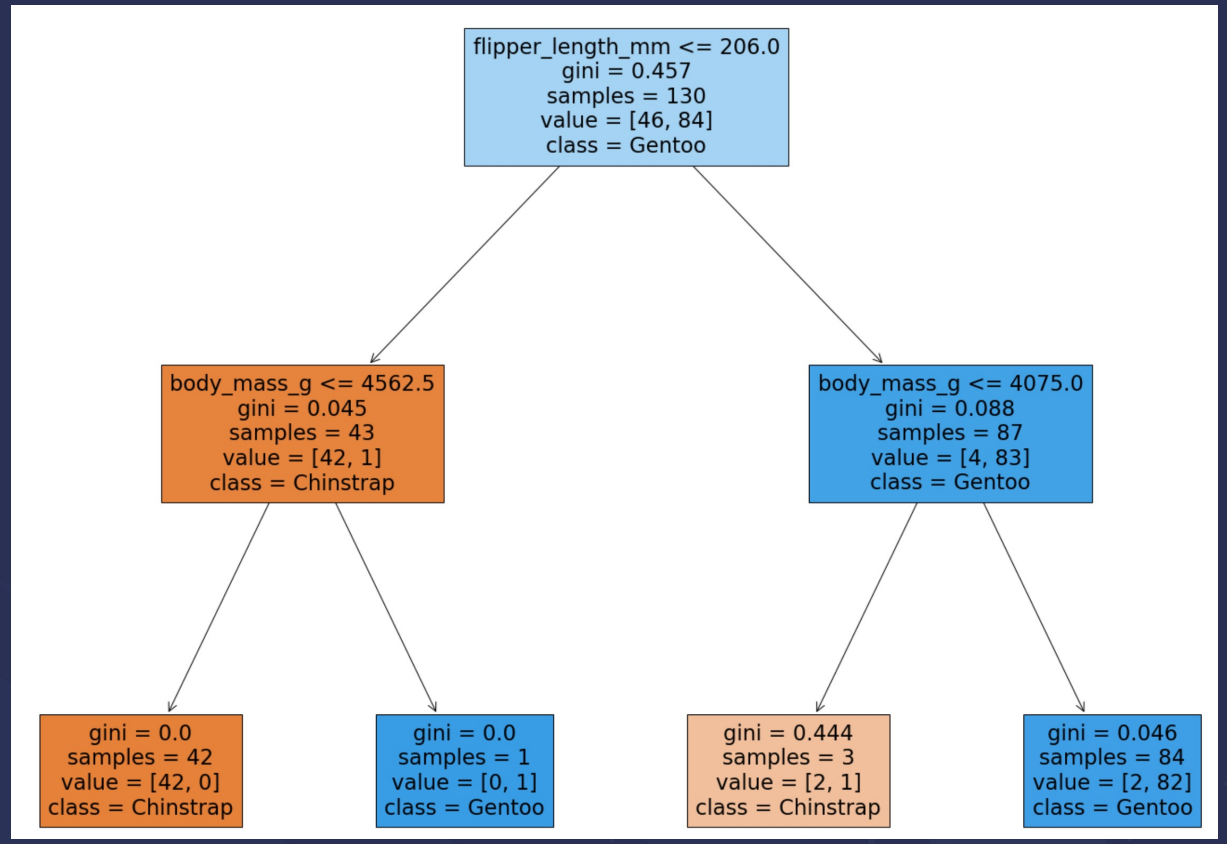
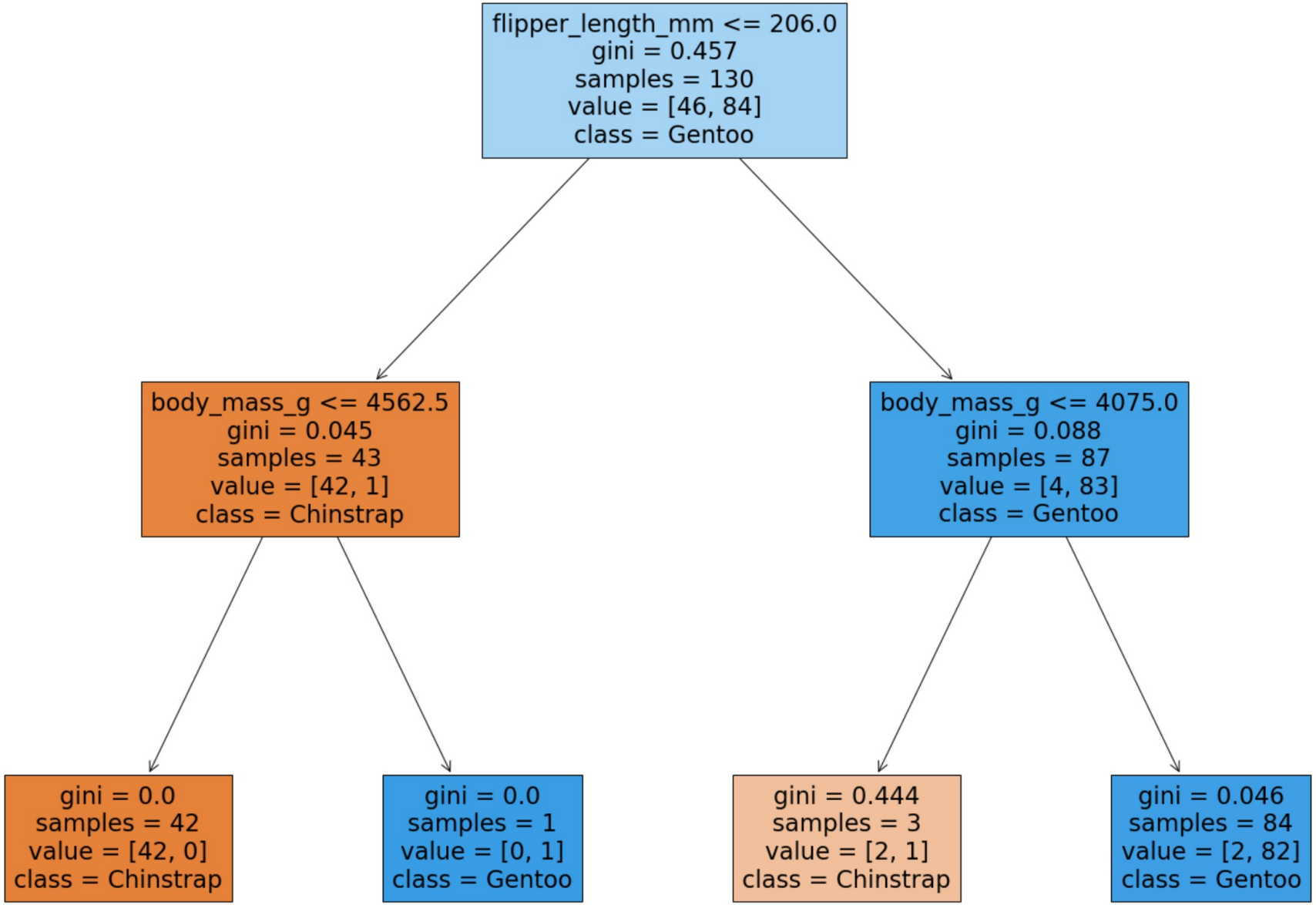
The inherent interpretability of ML models



Decision Tree Classifer



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Decision Tree Classifer

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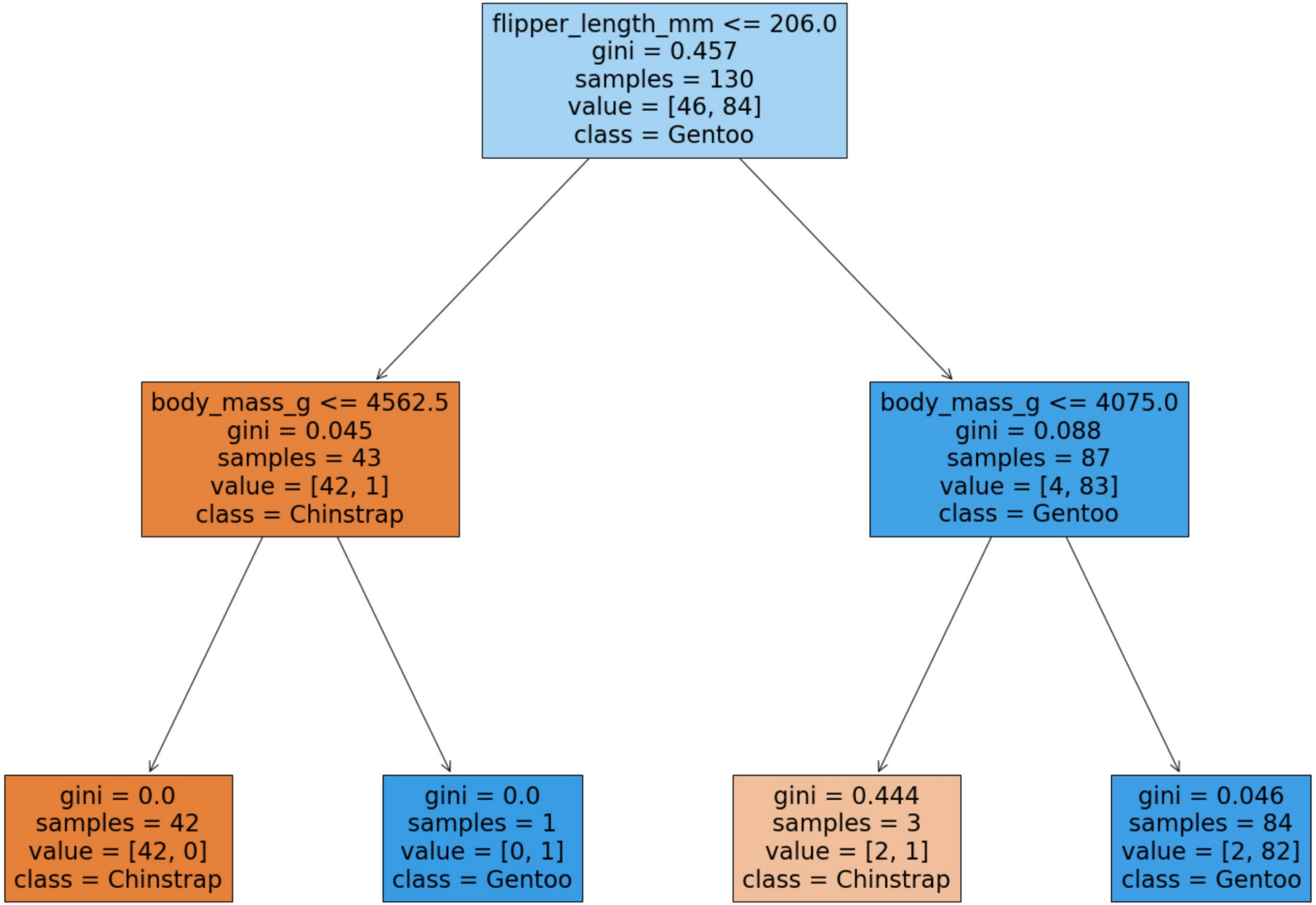
Decision Tree Classifer



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Decision Tree Classifer

gini = 0.457
samples = 130
value = [46, 84]
class = Gentoo

$$\text{gini} = 1 - \frac{46}{130}^2 - \frac{84}{130}^2 = 0.457\ldots$$

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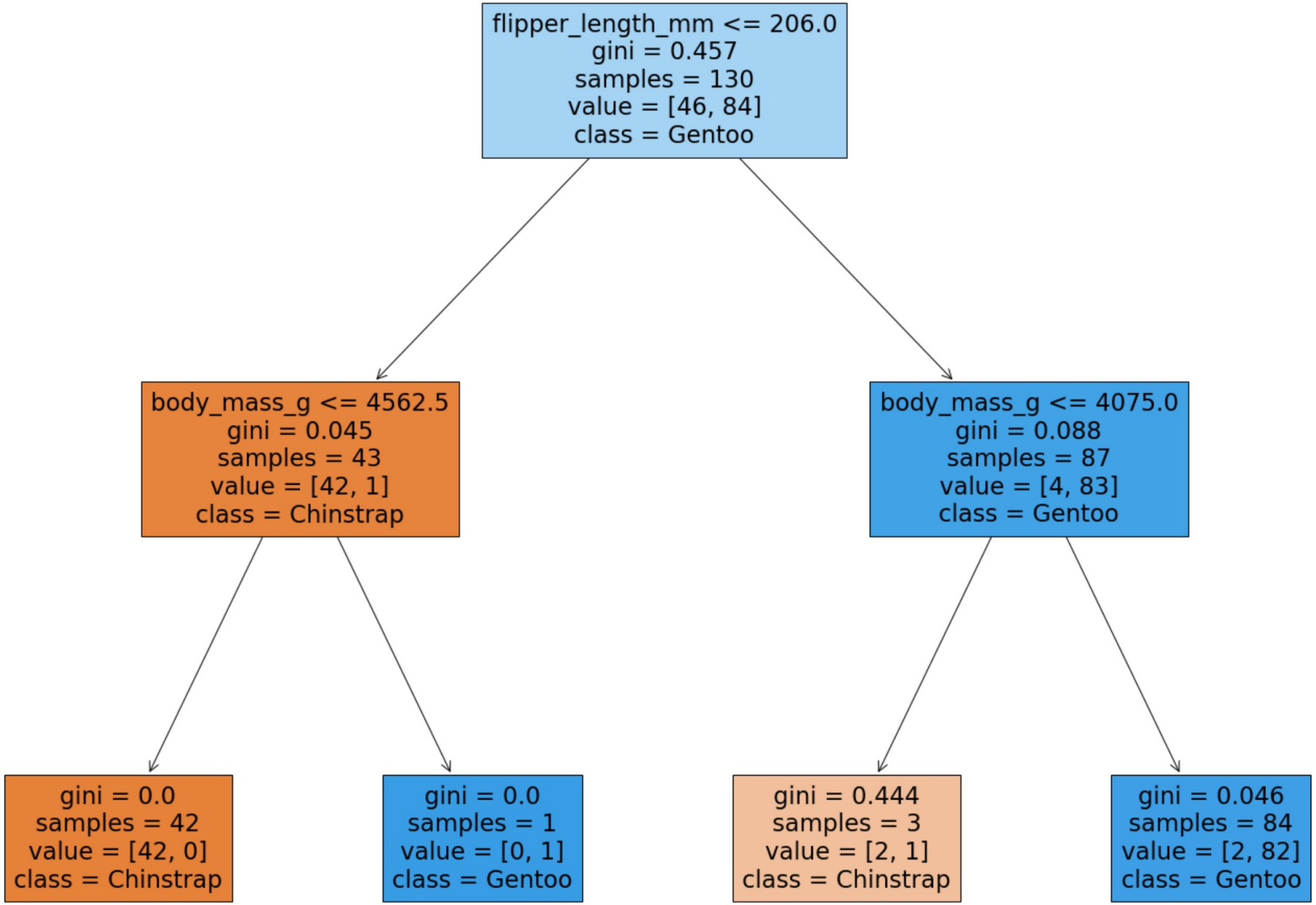
Decision Tree Classifer



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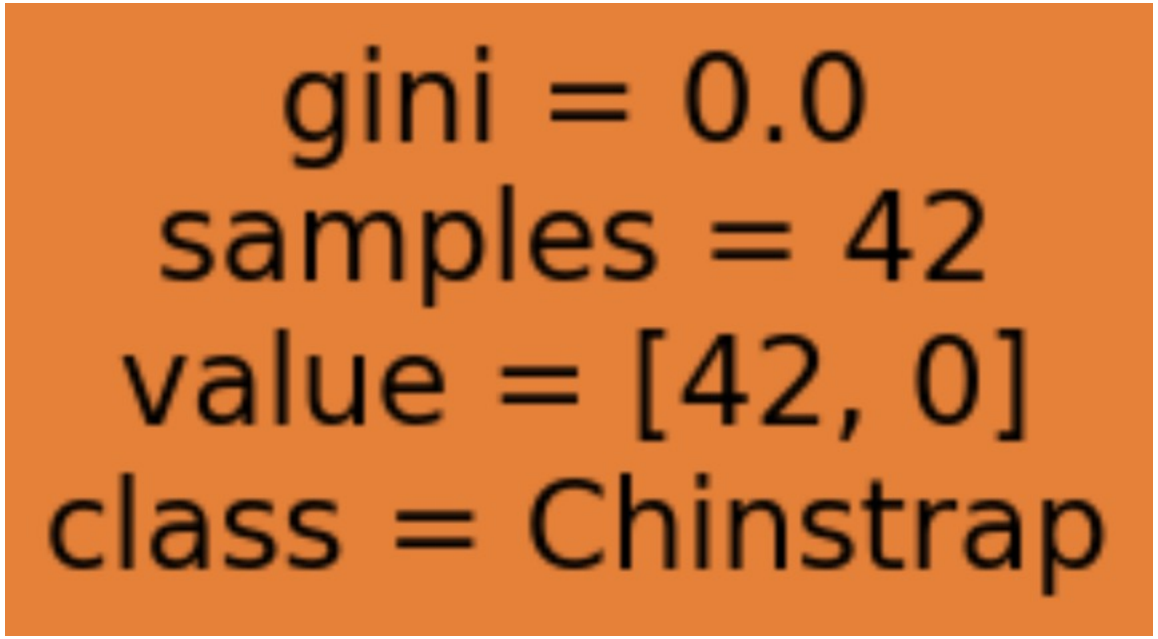
Decision Tree Classifer



$$\text{gini} = 1 - \frac{42}{42}^2 - \frac{0}{42}^2 = 1 - 1 - 0 = 1$$

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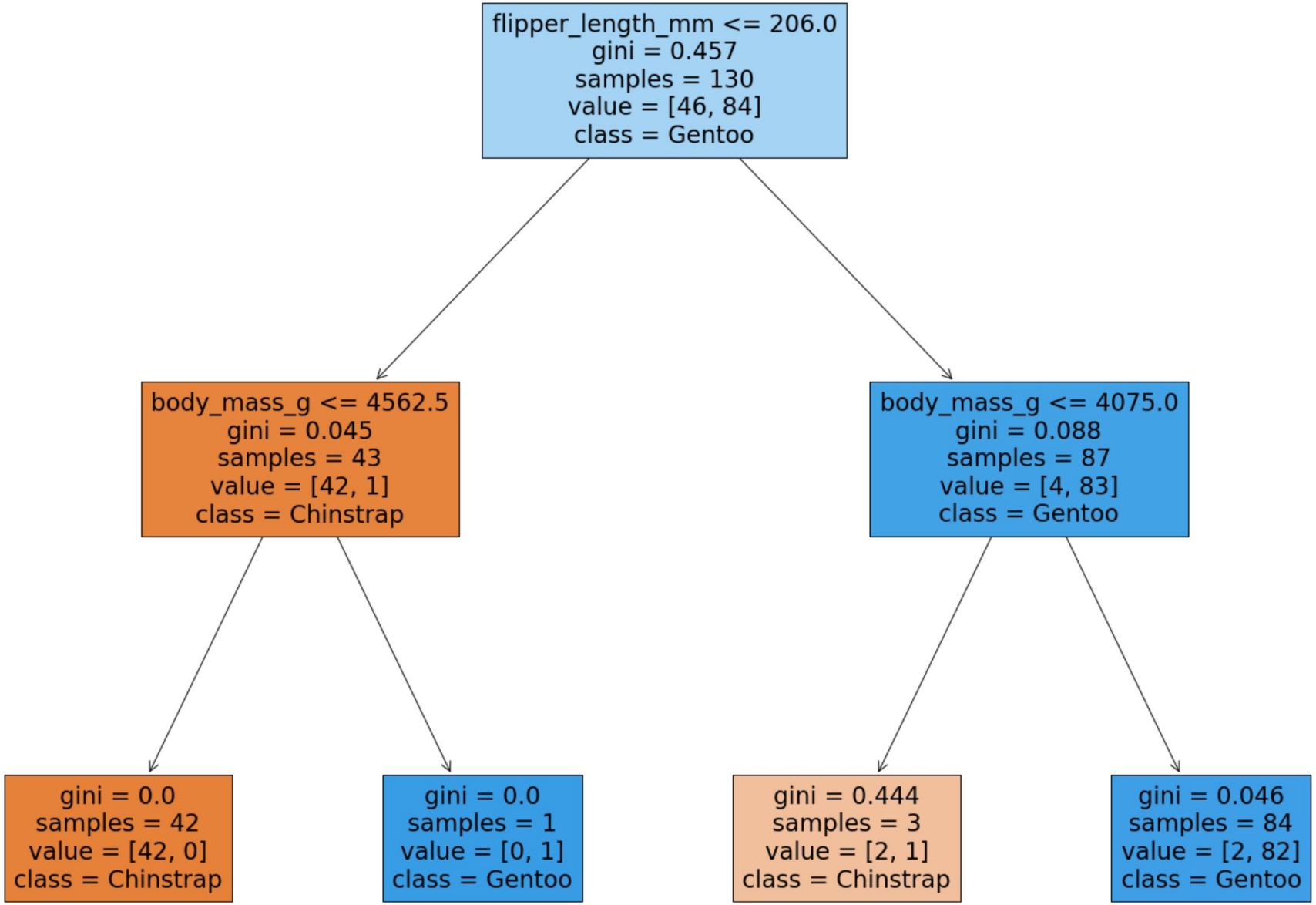
Decision Tree Classifer



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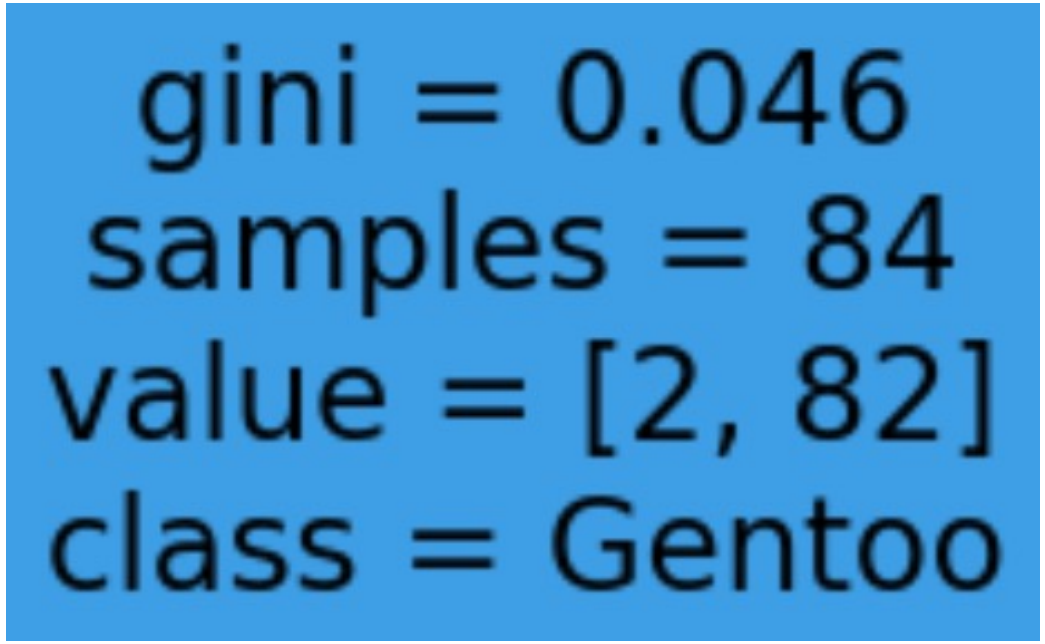
Decision Tree Classifer



$$\text{gini} = 1 - \frac{2}{84}^2 - \frac{82}{84}^2 = 0.046$$

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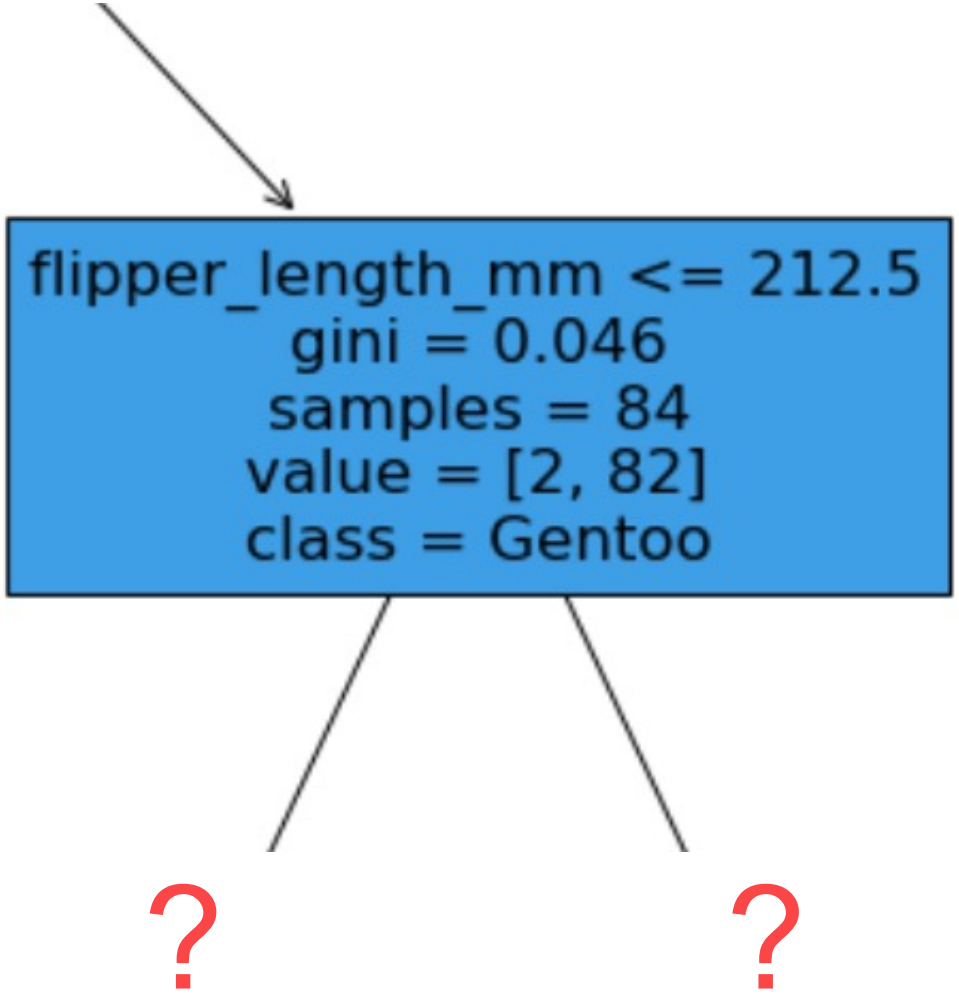
Decision Tree Classifer



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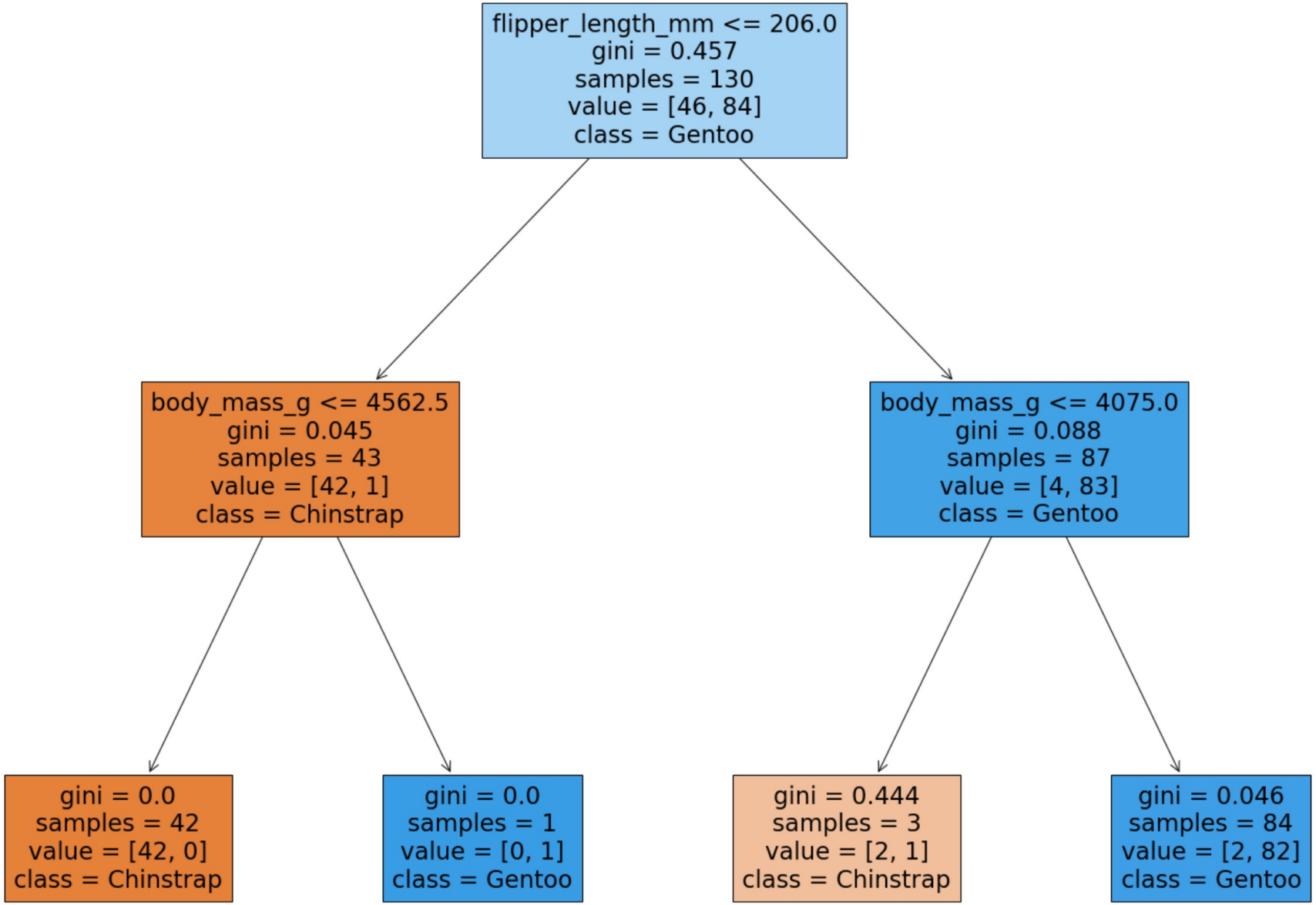
Decision Tree Classifer



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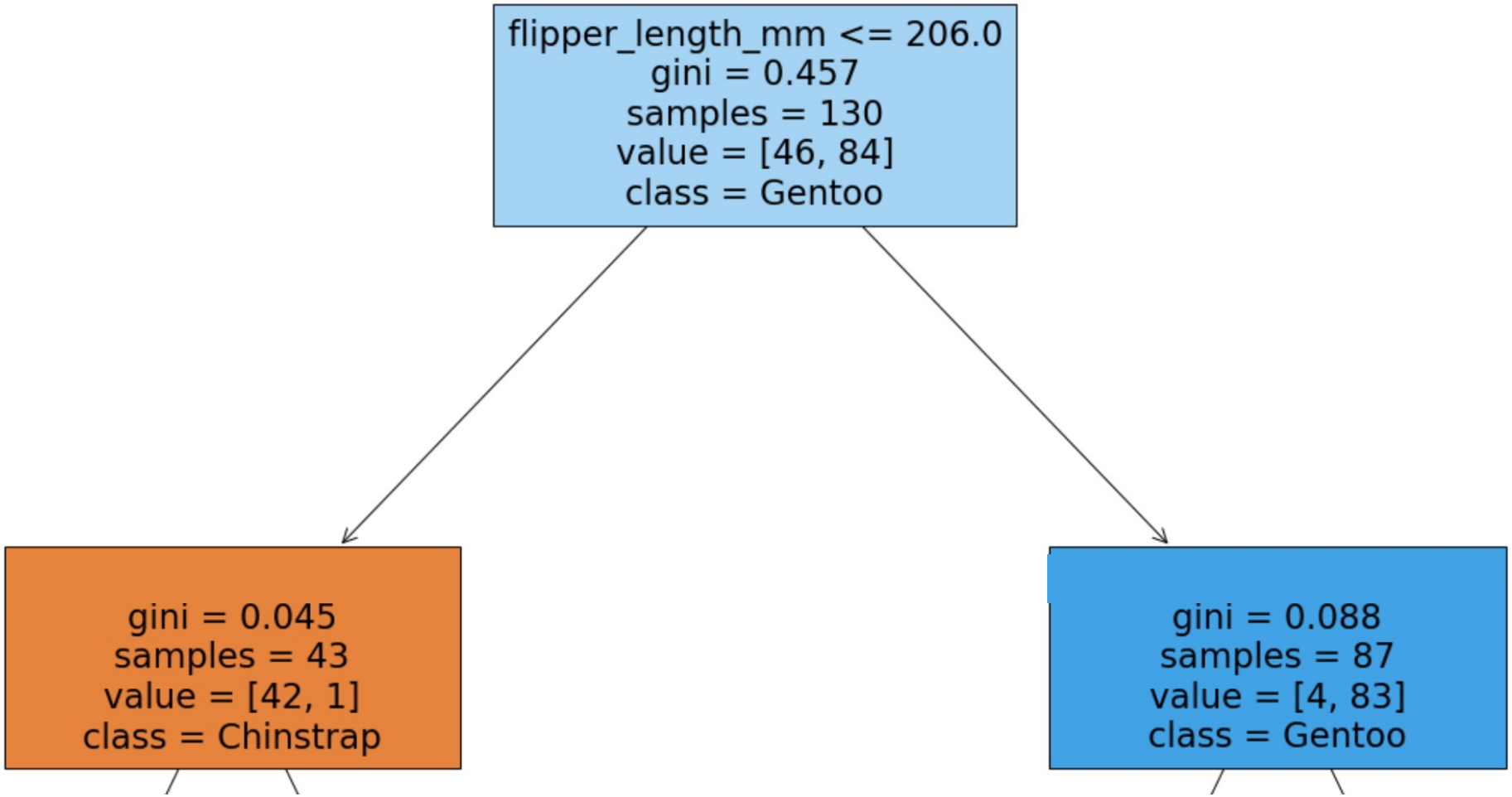
Decision Tree Classifer



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$$0.045 \times \frac{43}{130} + 0.088 \times \frac{87}{130} = 0.074$$

Penguin 218

- Flipper length: 210mm
- Body mass: 4100g

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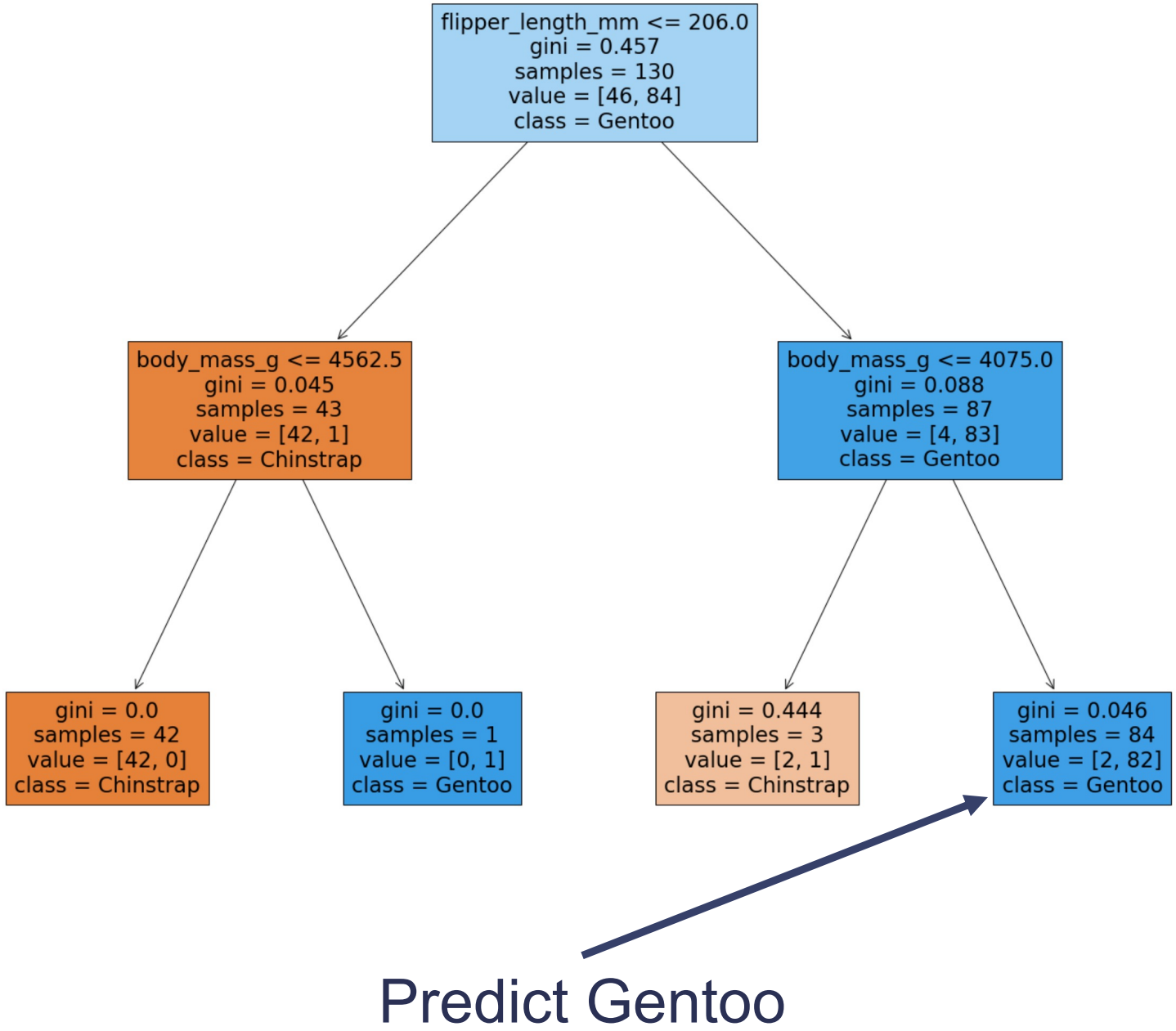
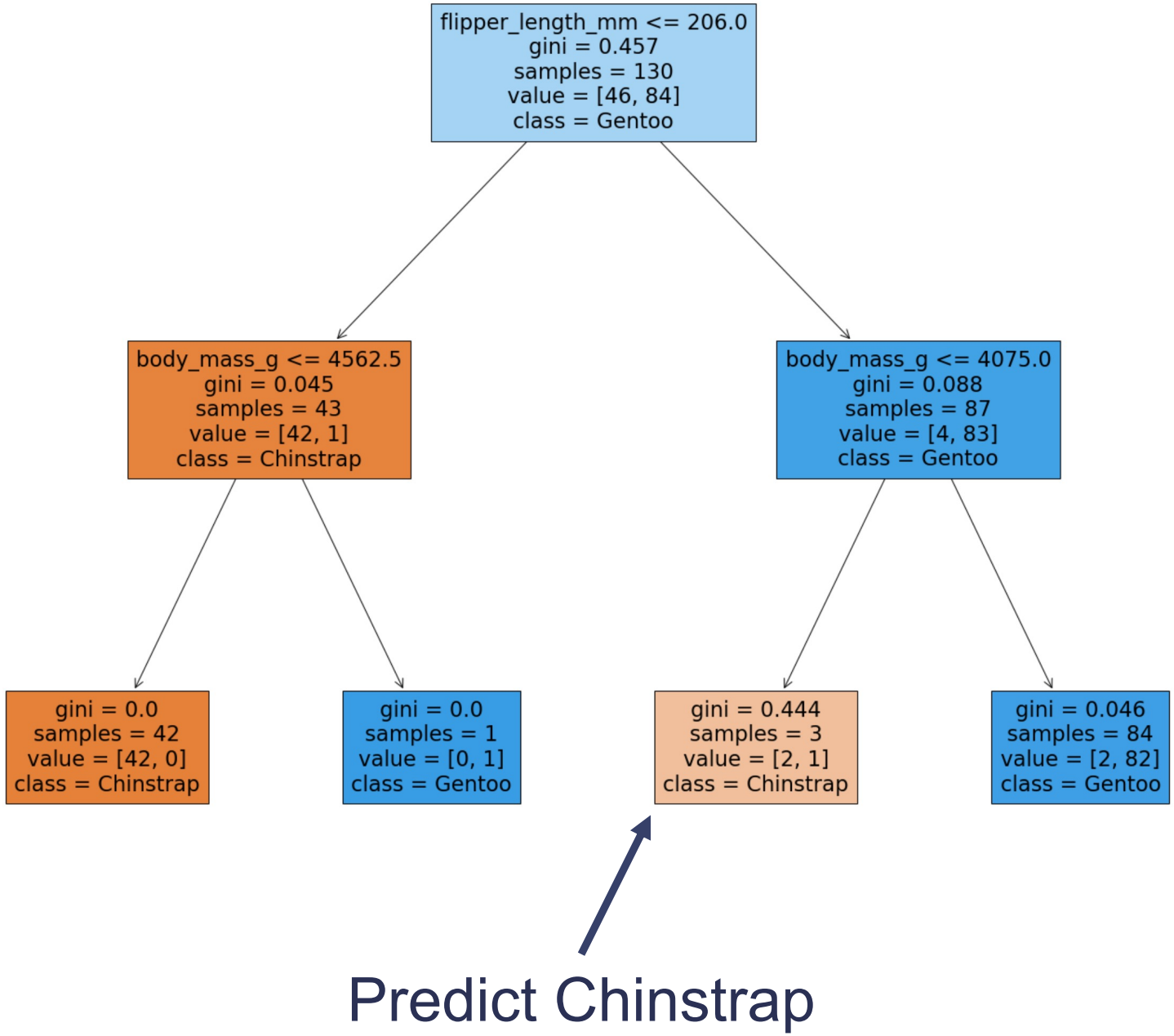


Penguin 218

- Flipper length: 210mm
- Body mass: 4070g

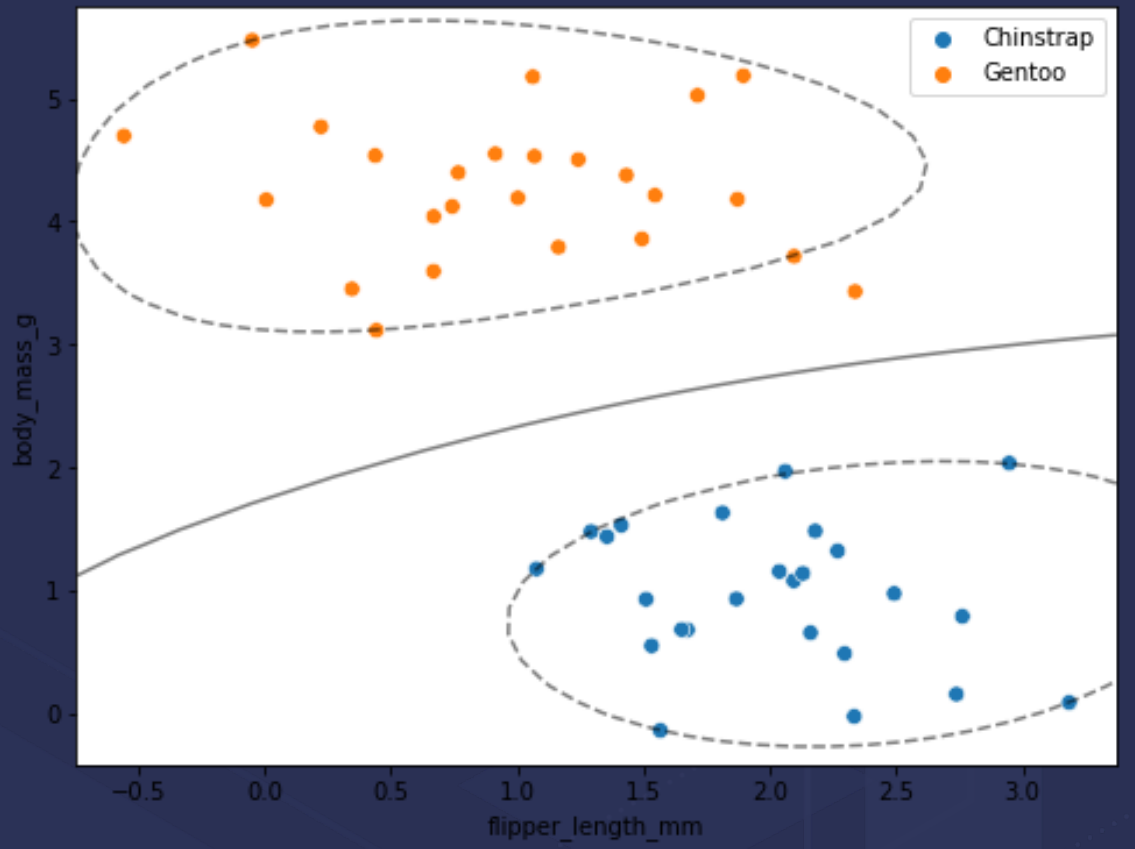
GO DATA DRIVEN



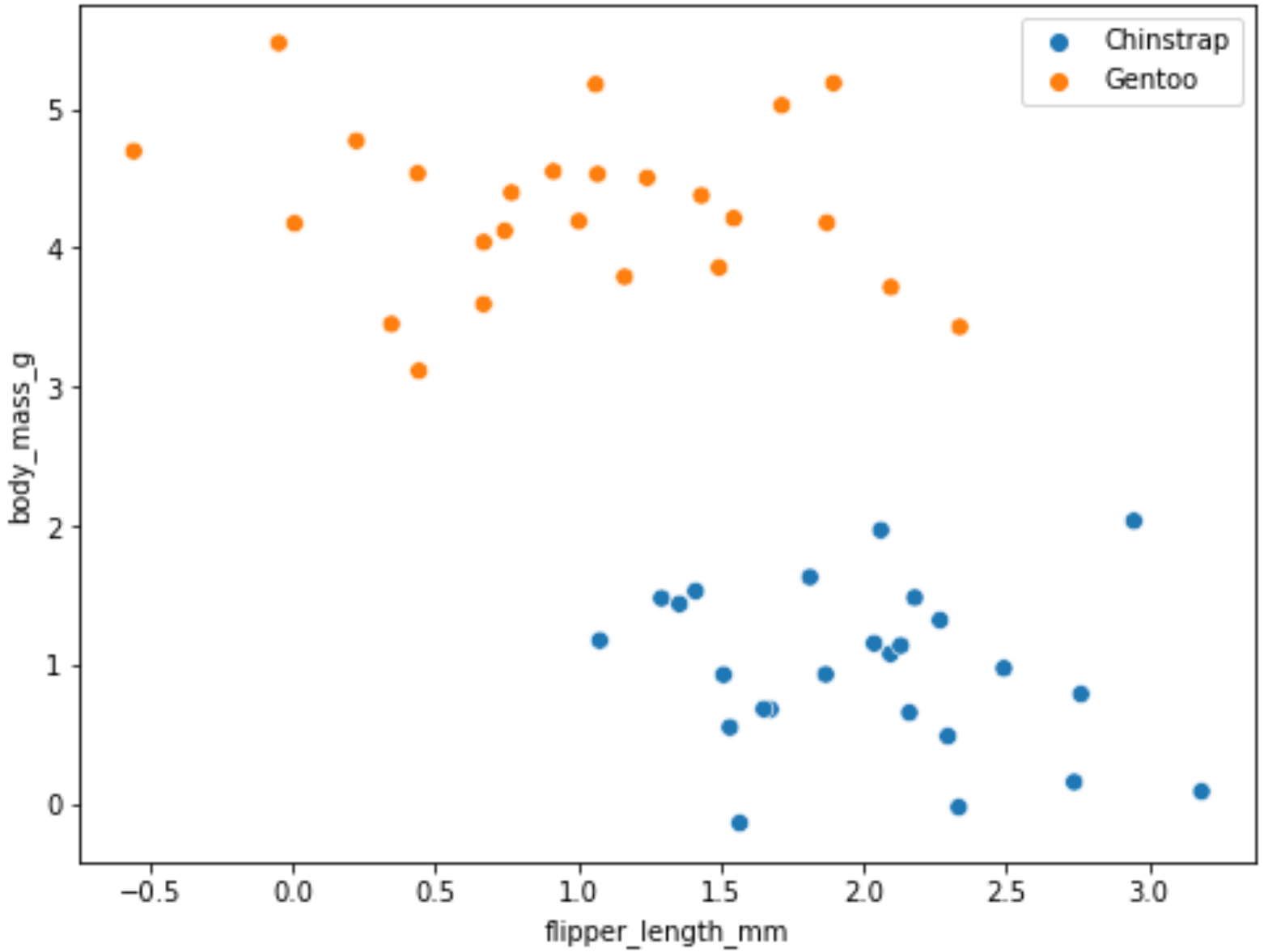
Support Vector Machine Classifer

GO DATA DRIVEN

The inherent interpretability of ML models

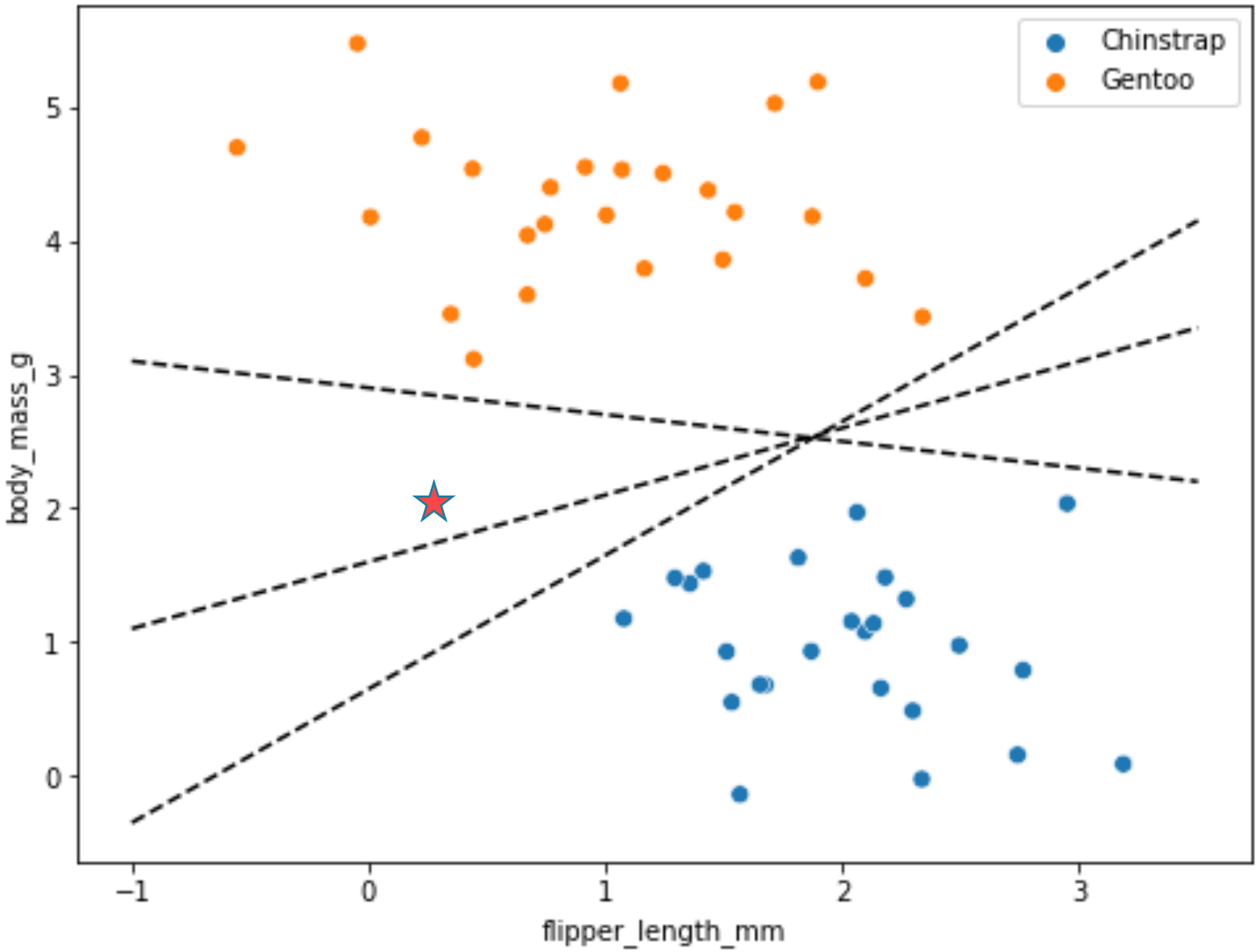


Support Vector Machine Classifier



GO DATA DRIVEN

Support Vector Machine Classifier



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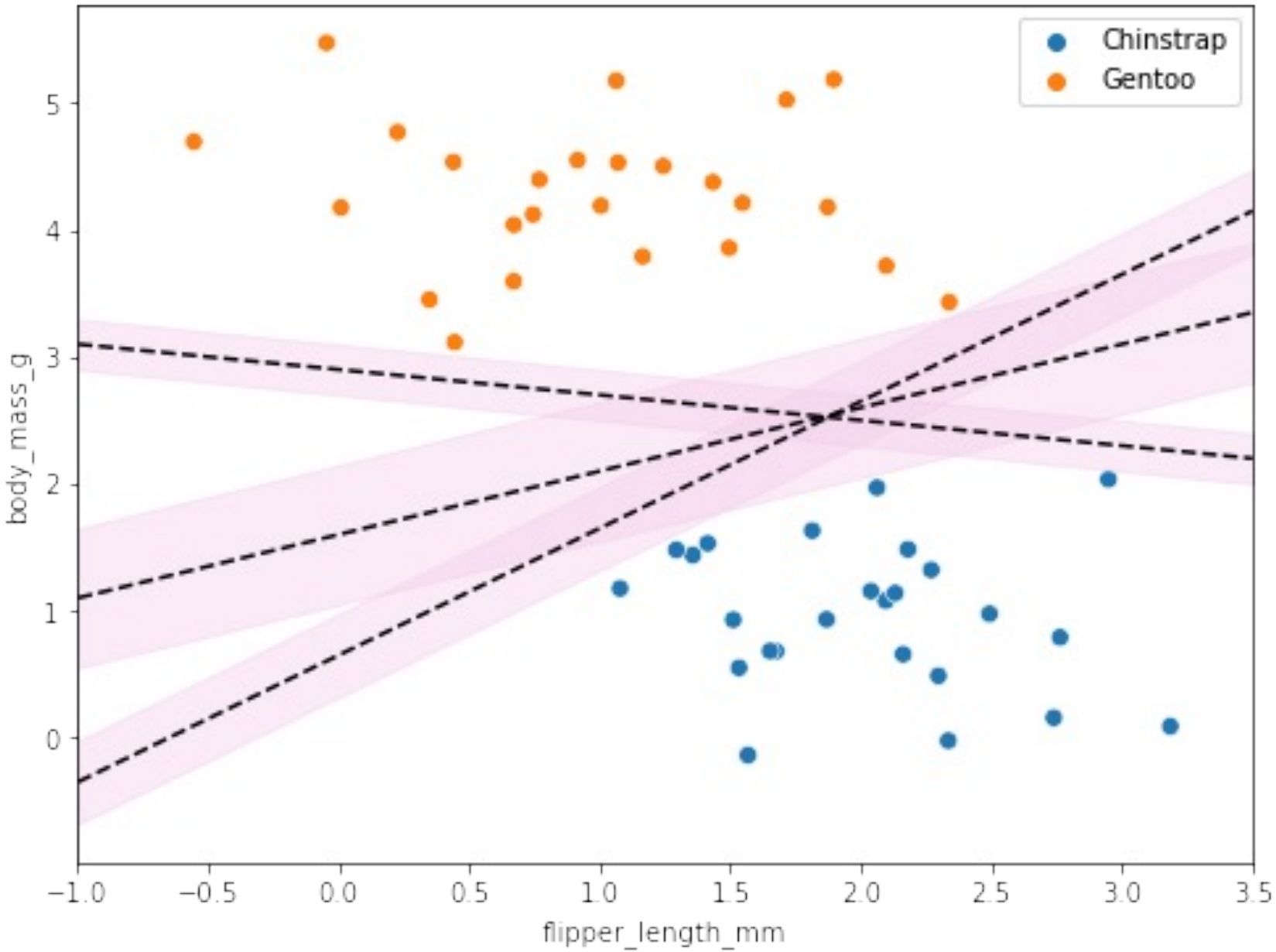
Support Vector Machine Classifier



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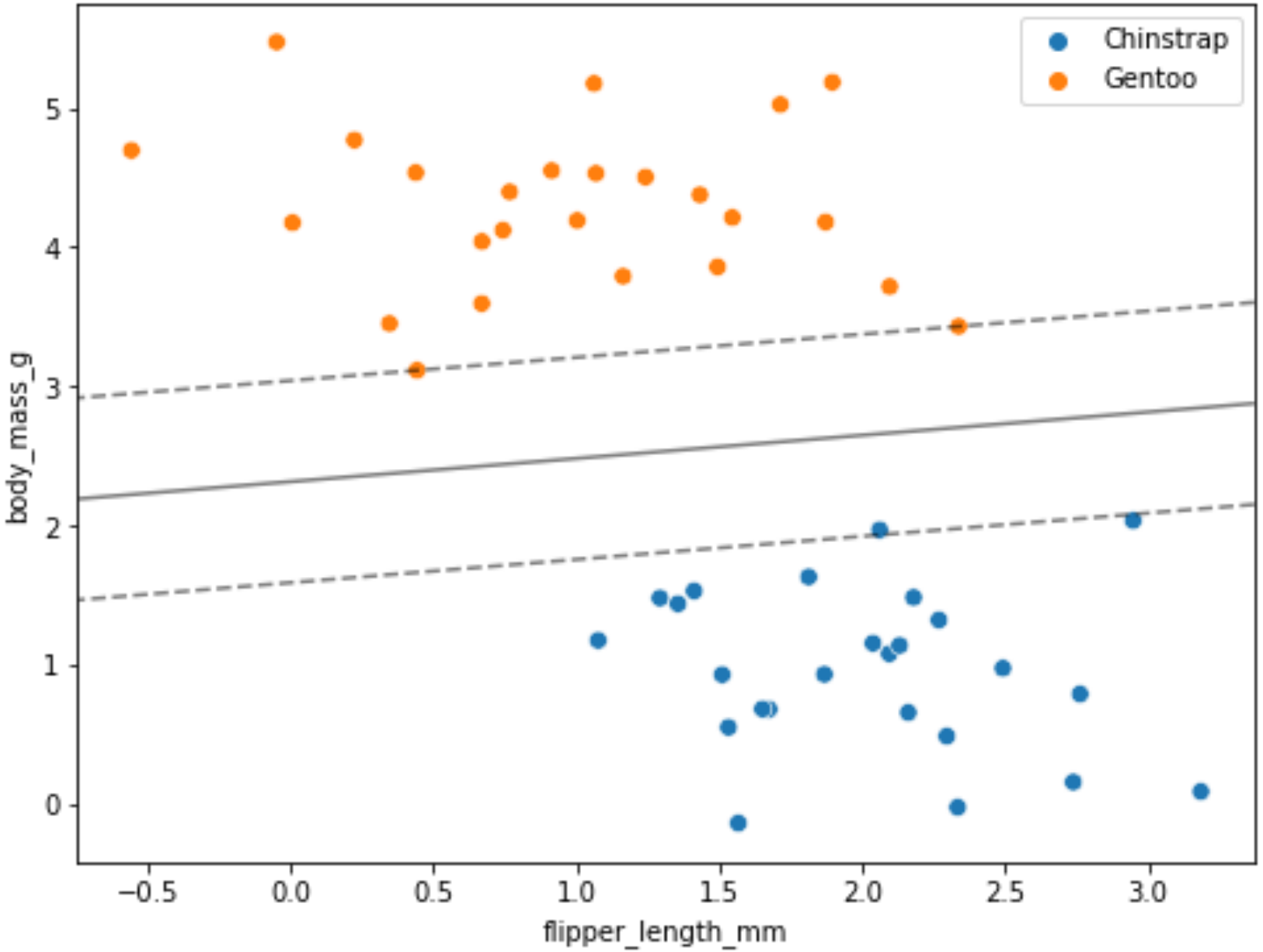
Support Vector Machine Classifier



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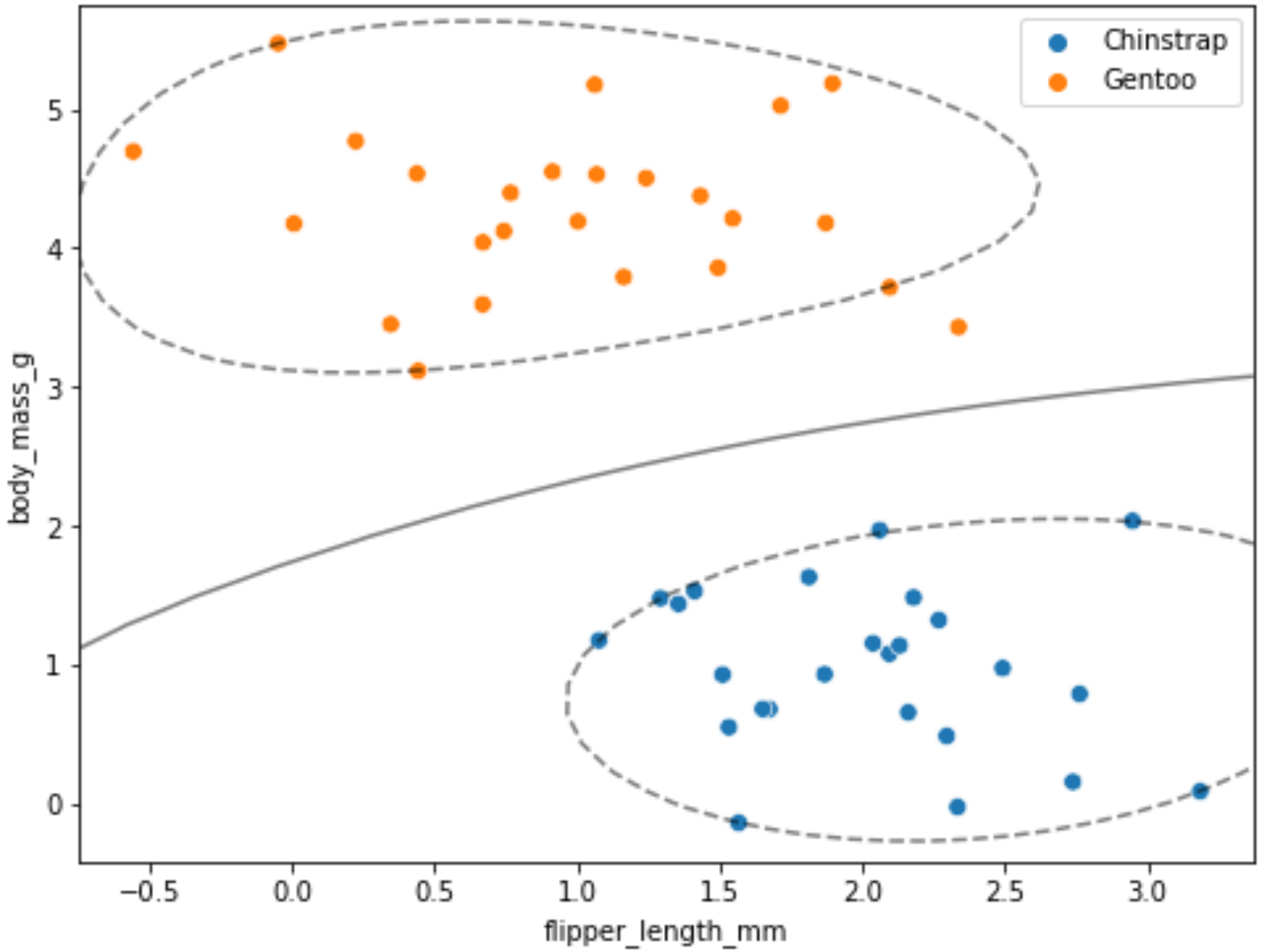
Support Vector Machine Classifier



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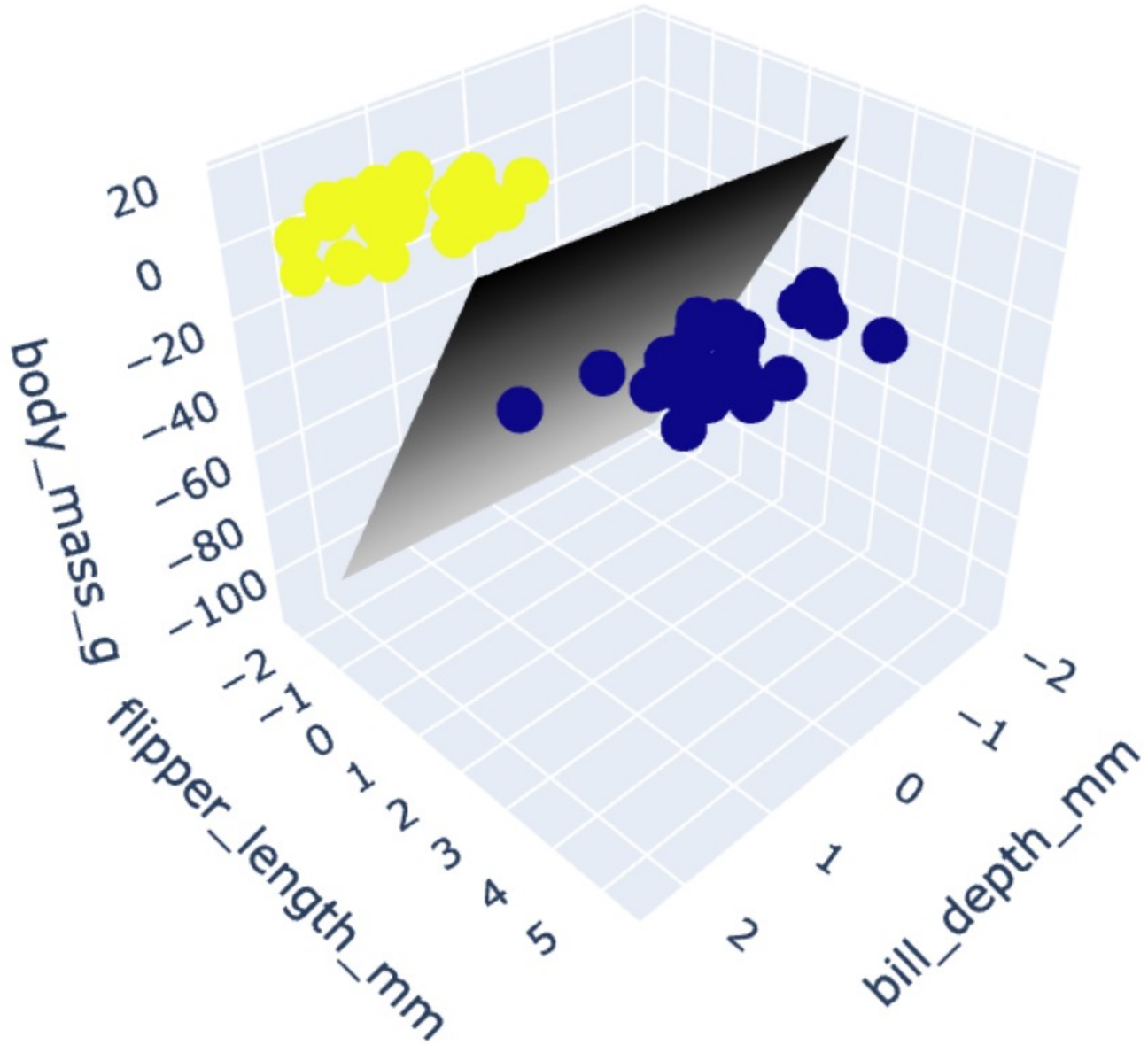
Support Vector Machine Classifier



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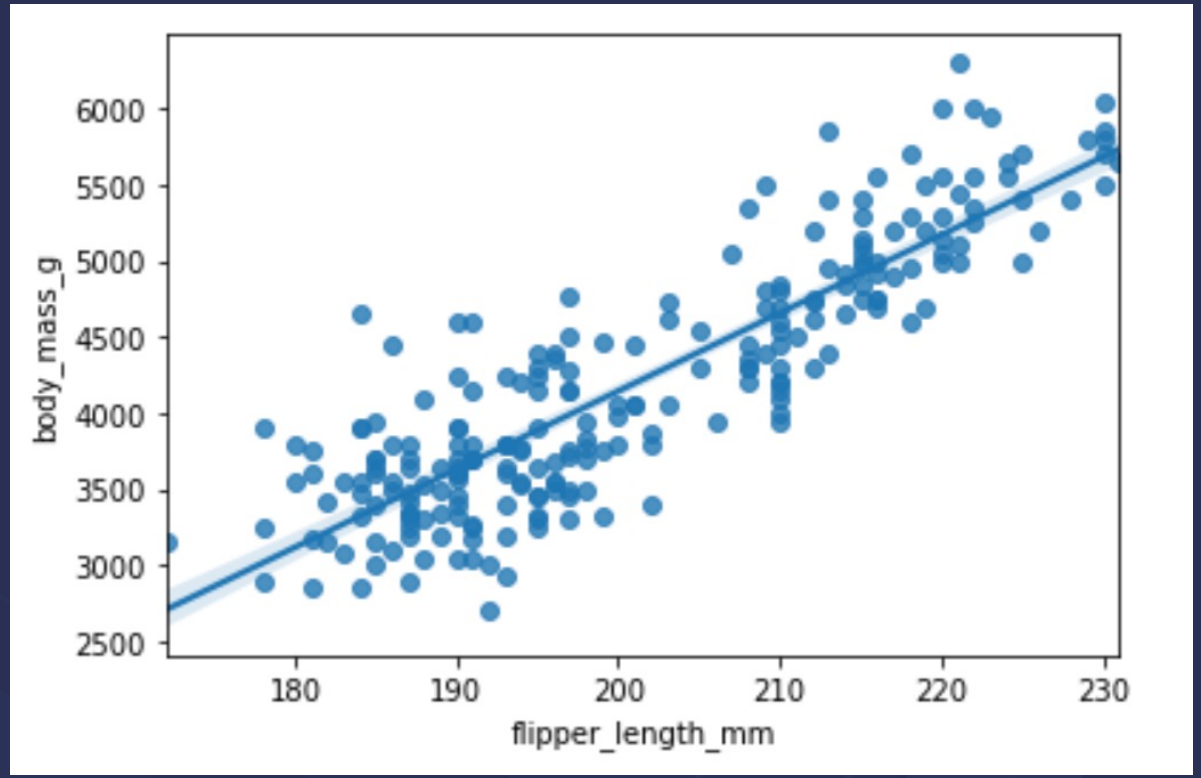
Linear Regression

The inherent interpretability of ML models



Classification

bill_depth_mm	flipper_length_mm	species
18.7	181.0	Adelie
17.4	186.0	Adelie
18.0	195.0	Adelie
19.3	193.0	Adelie
20.6	190.0	Adelie

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Regression

bill_depth_mm	flipper_length_mm	body_mass_g
18.7	181.0	3750.0
17.4	186.0	3800.0
18.0	195.0	3250.0
19.3	193.0	3450.0
20.6	190.0	3650.0

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Linear Regression

*m*bill depth + n*flipper length + c = body mass*

bill_depth_mm	flipper_length_mm	body_mass_g
18.7	181.0	3750.0
17.4	186.0	3800.0
18.0	195.0	3250.0
19.3	193.0	3450.0
20.6	190.0	3650.0

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Linear Regression

*m*bill depth + n*flipper length + c = body mass*

*14*bill depth + 53*flipper length - 6600 = body mass*

bill_depth_mm	flipper_length_mm	body_mass_g
18.7	181.0	3750.0

*14*18.7+ 53*181.0 - 6600 = 3171*

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Model-agnostic interpretability methods

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Jupyter Notebook 2

02_Ceteris_Paribus_Plots.ipynb

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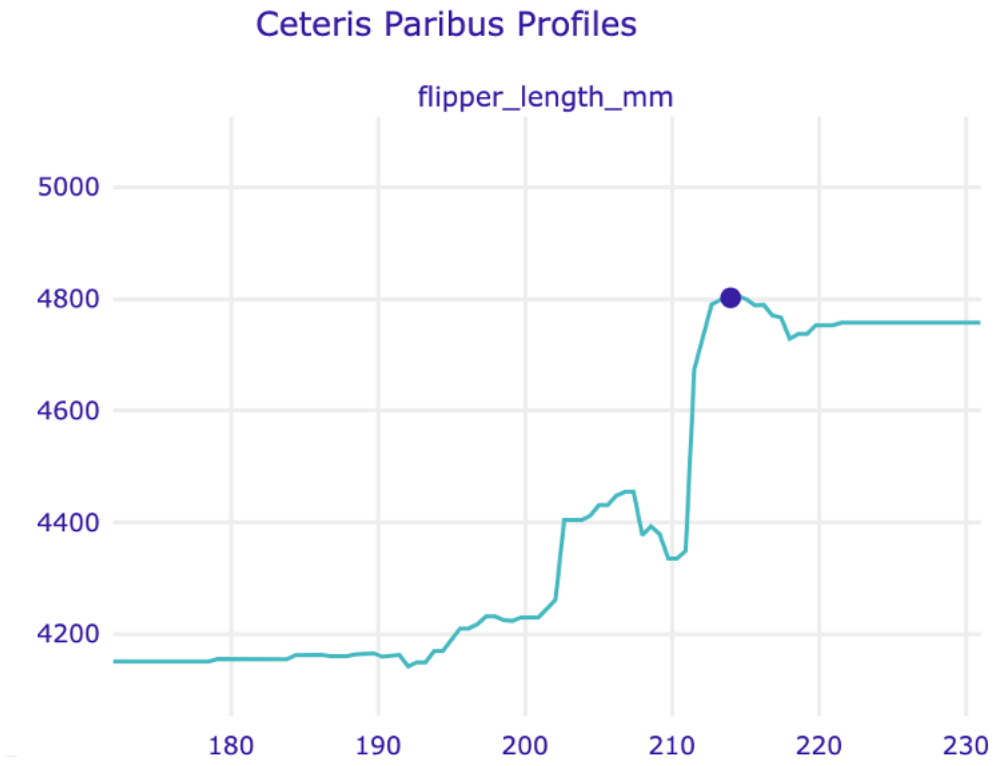
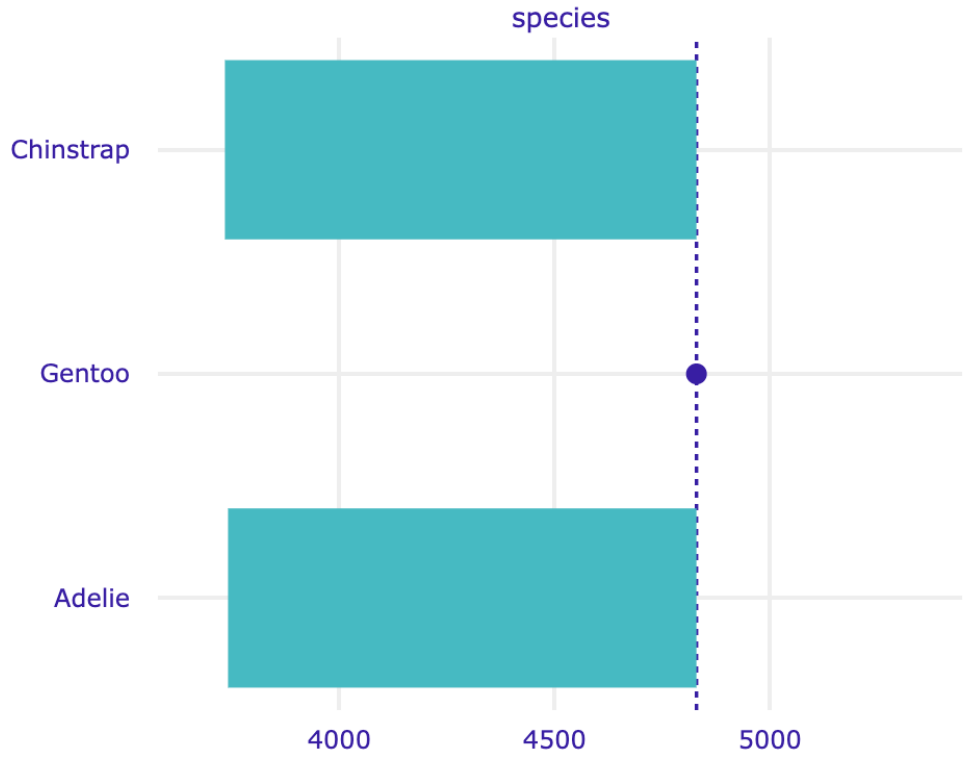
Ceteris Paribus profile

Numerical and categorical features



Numerical features



Categorical features

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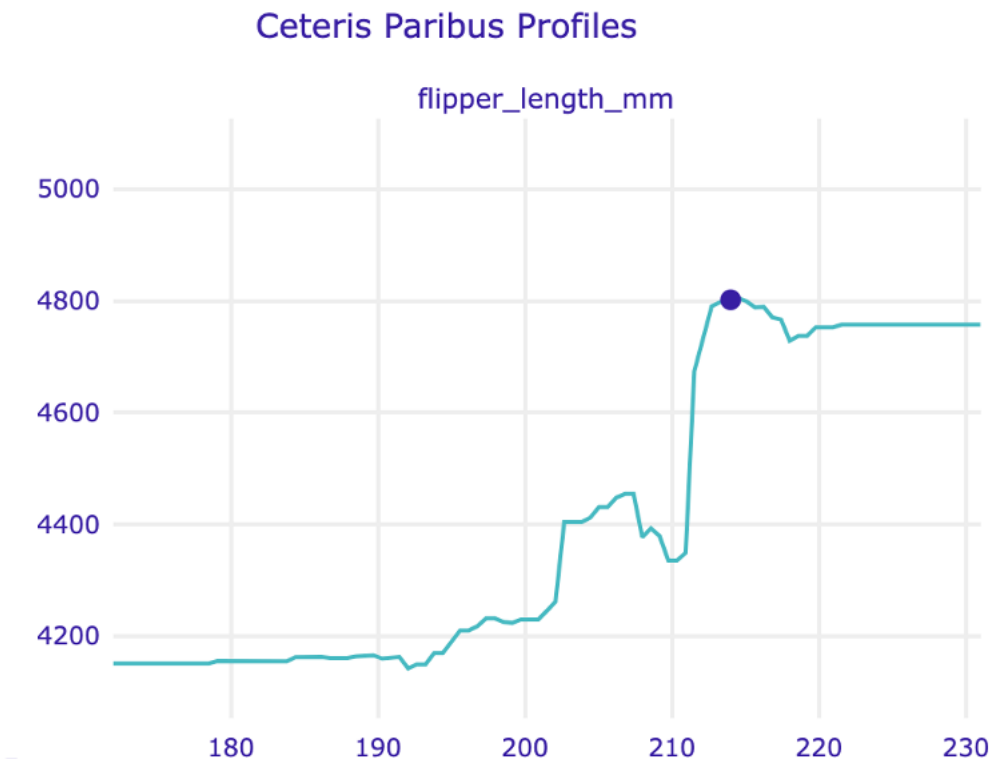
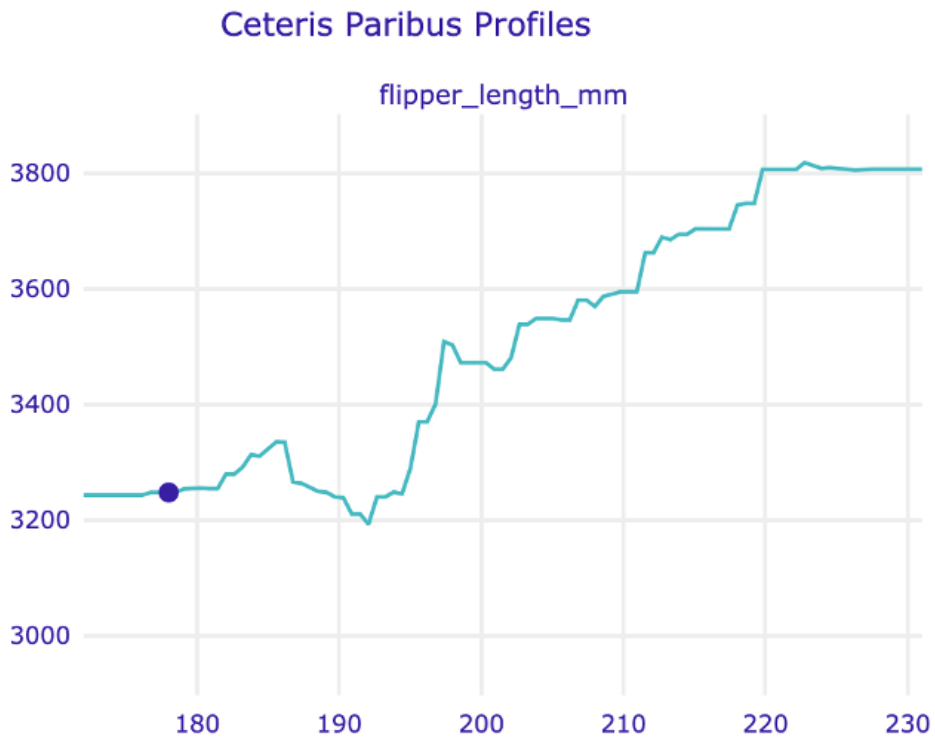
Ceteris Paribus profile

Different plots for different *data points*



Row 231: A Gentoo penguin

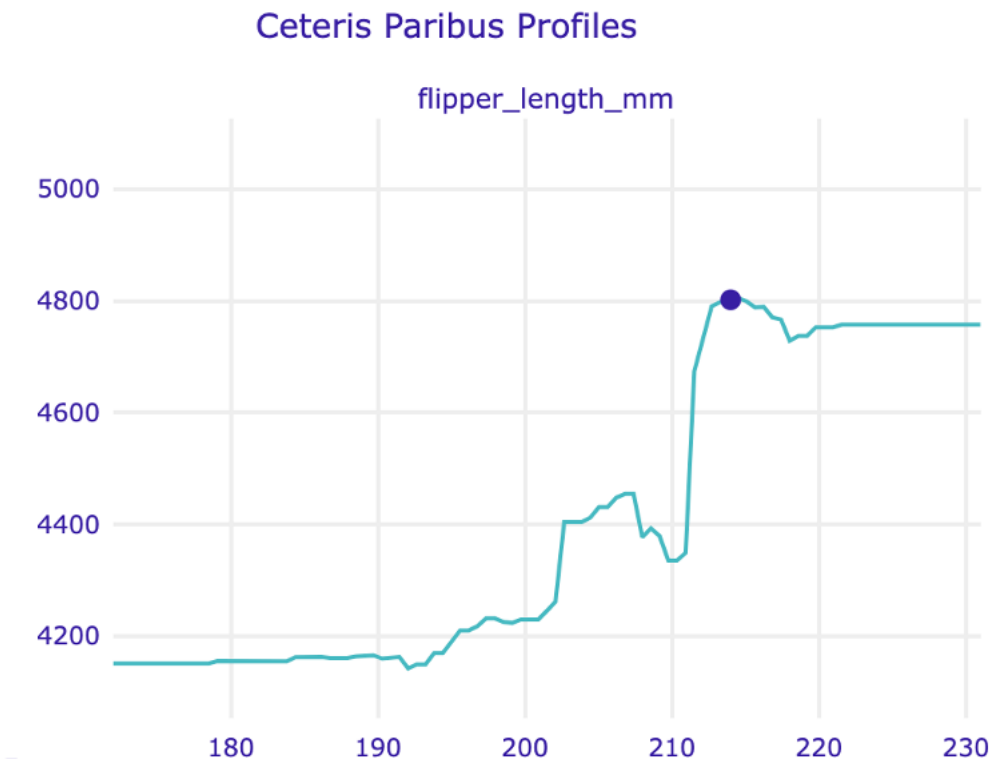


Row 30: An Adélie penguin

GO DATA DRIVEN

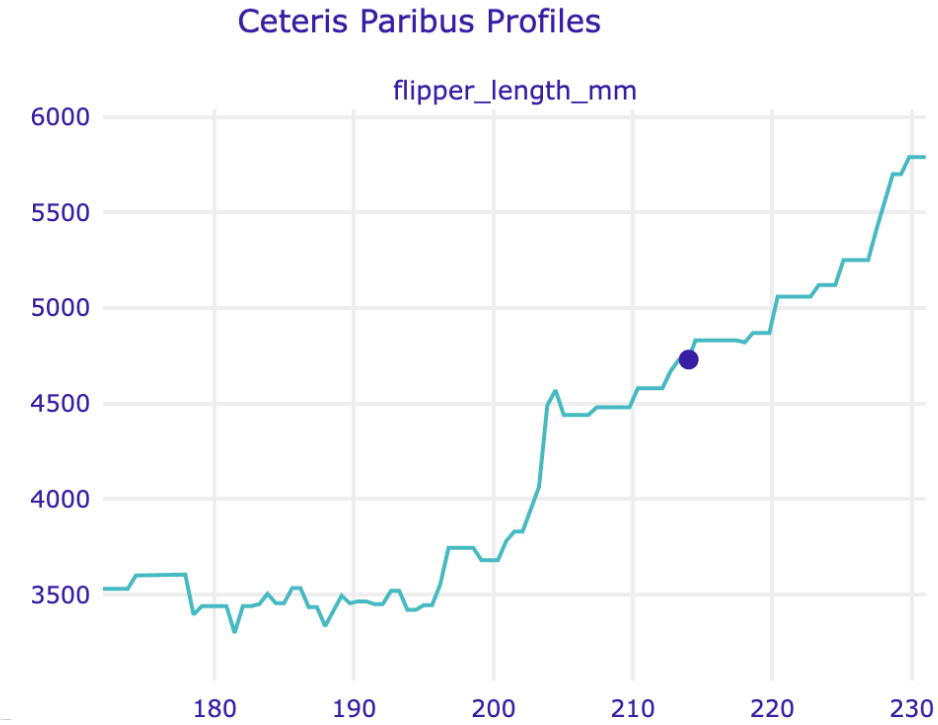
Ceteris Paribus profile

Different plots for different *models*



Row 231: A Gentoo penguin

Random Forest Regressor



Row 231: A Gentoo penguin

K-Nearest Neighbors Regressor

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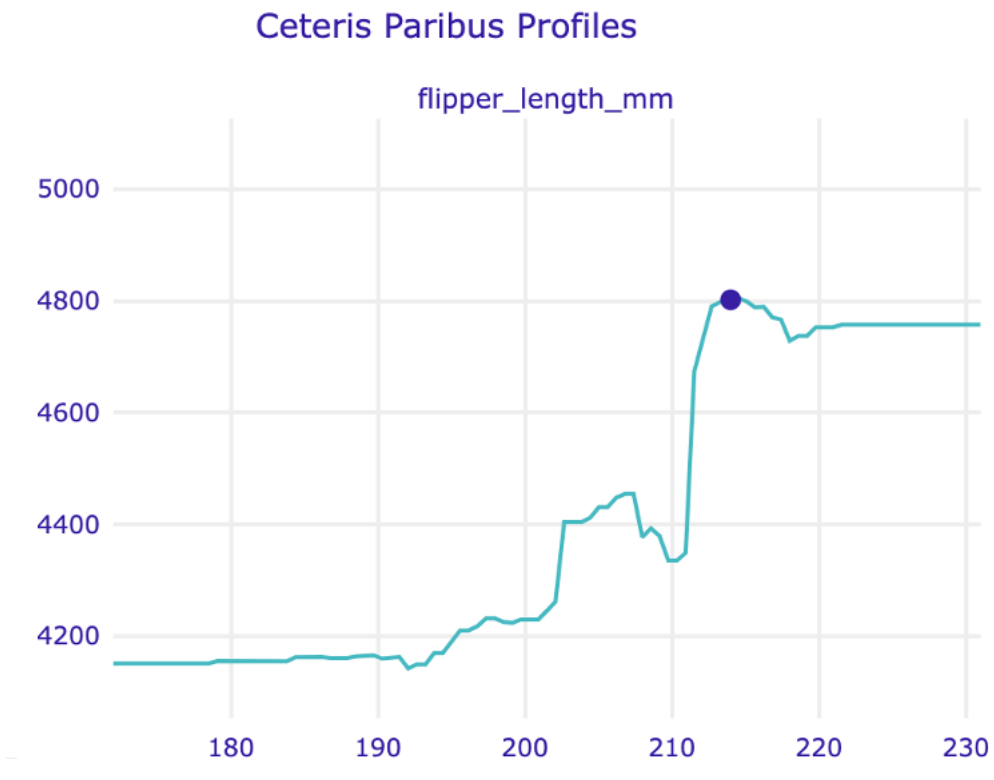
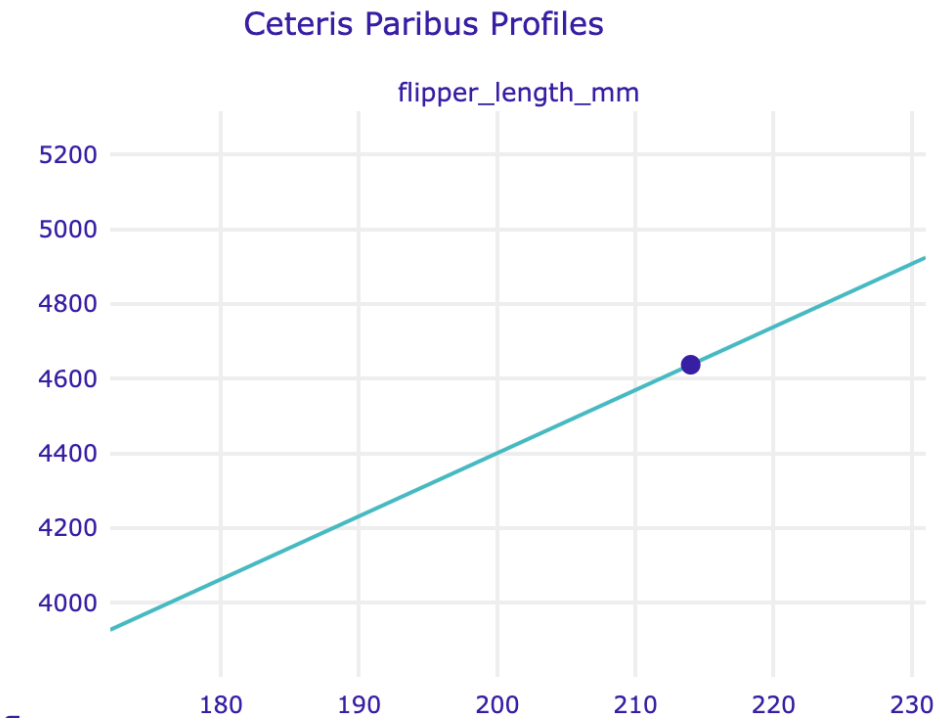
Ceteris Paribus profile

Different plots for different *models*



Row 231: A Gentoo penguin

Random Forest Regressor



Row 231: A Gentoo penguin

Linear Regression

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Ceteris Paribus profile

Advantages

- Works on a **local** level for an individual prediction
- Displays model's **sensitivity** to a feature
- **Intuitive** to understand
- (**Easy** to implement)

Disadvantages

- Can only display **one feature** meaningfully at the time
- Misleading for **correlated** features
- Only applicable to **one** data point at the time – does not tell you anything about overall trend
- Does not tell you **how much a feature contributes** to individual prediction

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Jupyter Notebook 3

03_Prediction_Break_Down.ipynb

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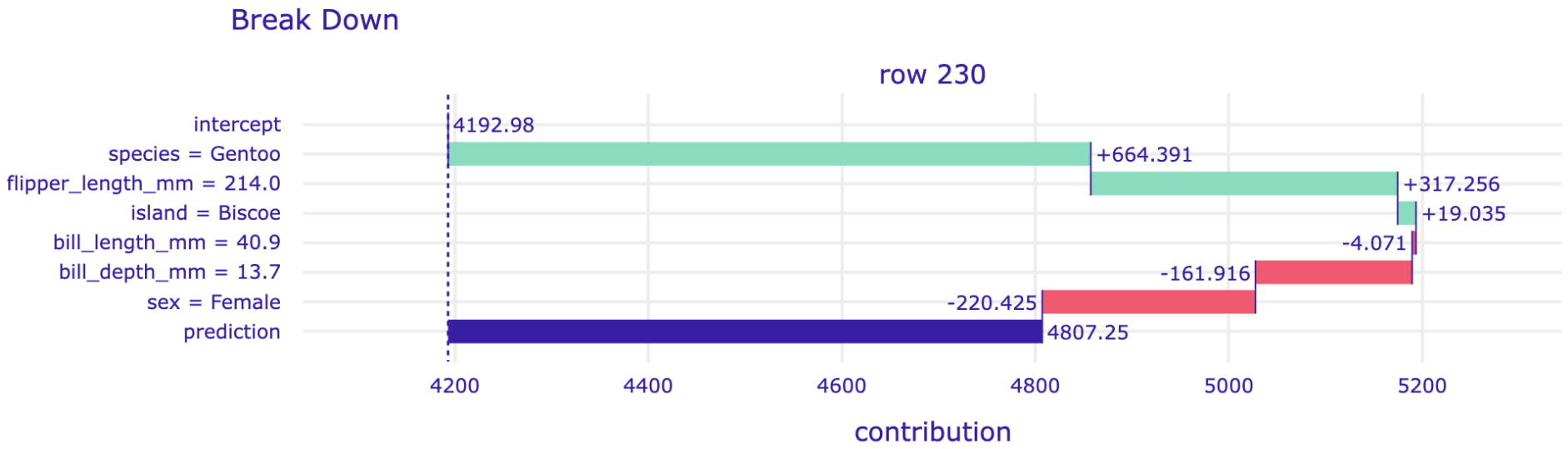
Break-down Plots for Additive Attributions

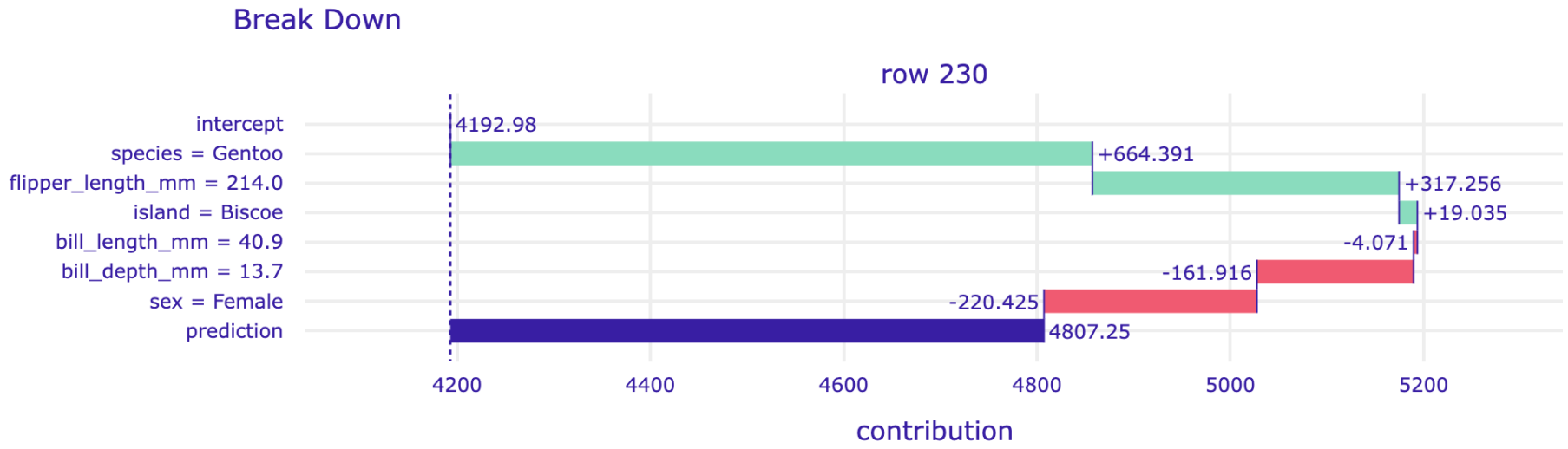


How to calculate the intercept:

1. Generate predictions with the model on the **train set** `y_hat = model.predict(X_train)`
2. Calculate the **average prediction** on the train set `intercept = y_hat.mean()`

GO DATA DRIVEN

Break-down Plots for Additive Attributions



How to calculate the value for *species = Gentoo*:

1. Assume that **all** datapoints in your dataset have the value Gentoo

```
X_train['species'] = 'Gentoo'
```

2. Calculate the **average prediction** on the altered (!) train set

```
value = model.predict(X_train).mean()
```

3. Subtract the intercept

```
value - intercept
```

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Ceteris Paribus profile

Advantages

- Works on a **local** level for an individual prediction
- Displays a feature's **importance**
- **Fast** to calculate
- **Visual**

Disadvantages

- The **order** of the features matters
- Misleading for **interactions**
- **Messy** for many variables
- Does not tell you how **sensitive** a model is to a feature
- Only applicable to **one** data point at the time – does not tell you anything about feature importance

GO DATA DRIVEN

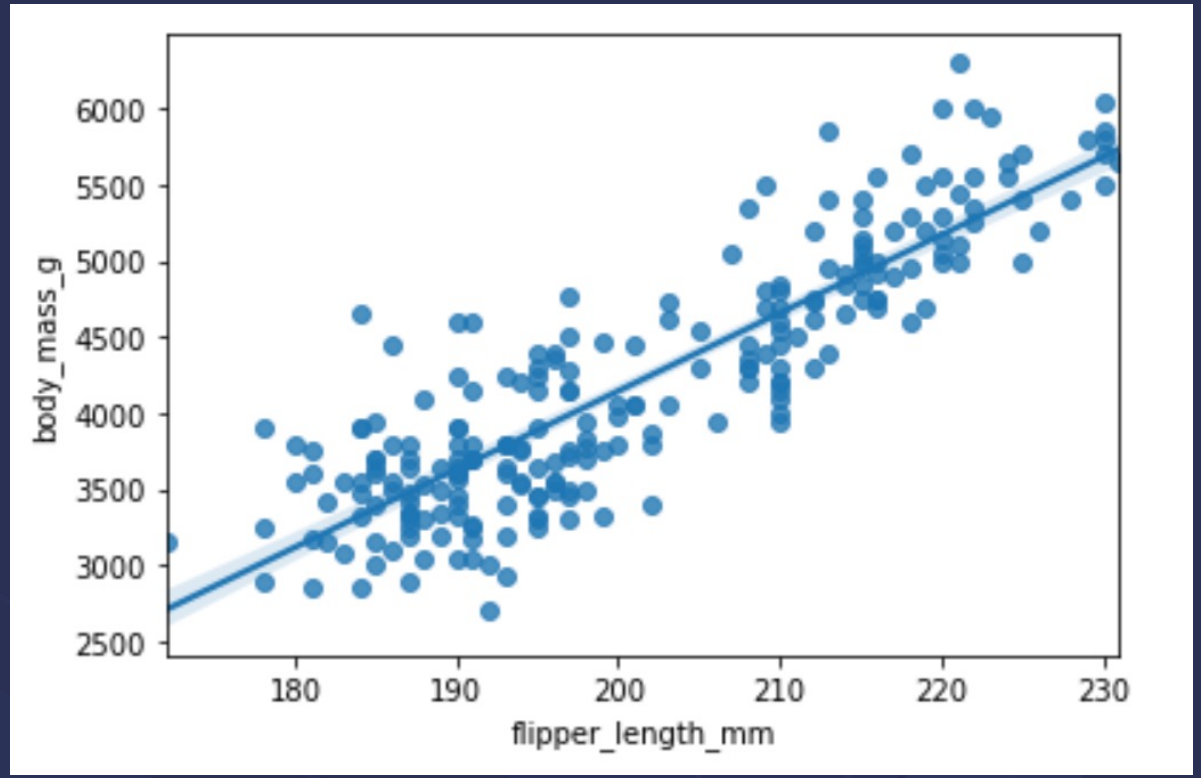
Global Feature Importance

GO DATA DRIVEN

Linear Regression

GO DATA DRIVEN

Global feature impotances



Linear Regression

*m*bill depth + n*flipper length + c = body mass*

*14*bill depth + 53*flipper length - 6600 = body mass*

bill_depth_mm	flipper_length_mm	body_mass_g
18.7	181.0	3750.0

*14*18.7+ 53*181.0 - 6600 = 3171*

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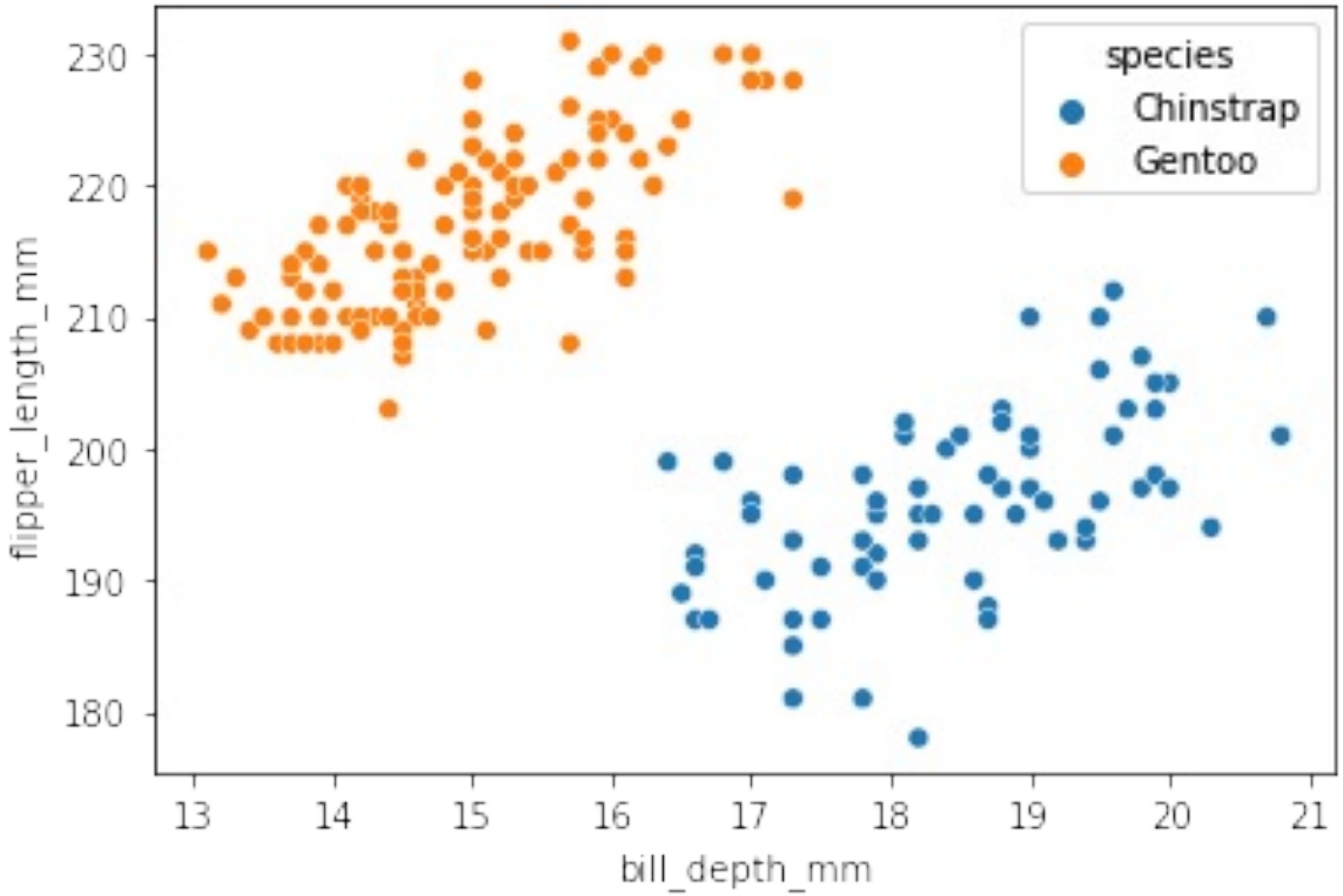
Linear Regression

*14*bill depth + 53*flipper length - 6600 = body mass*



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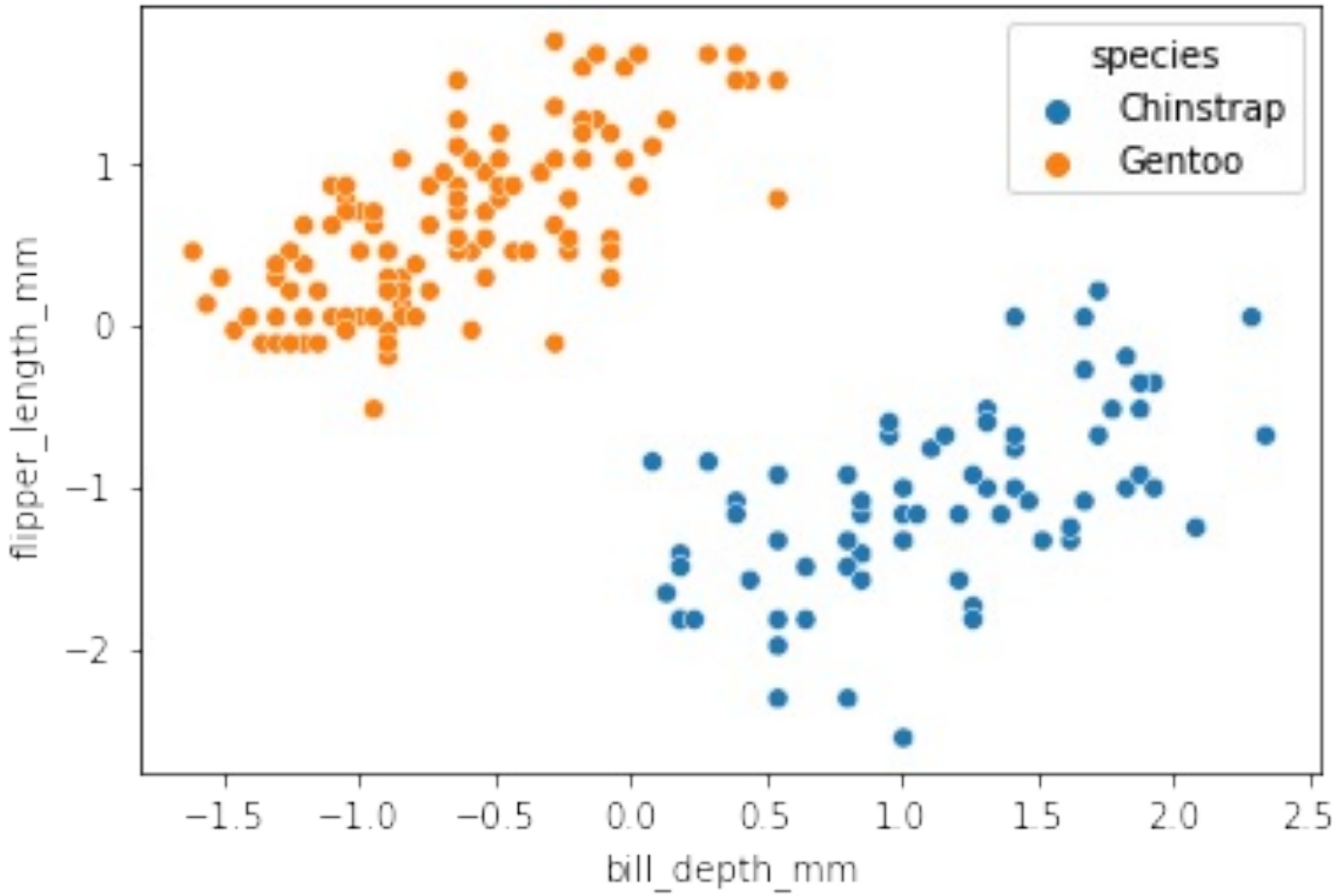
Linear Regression



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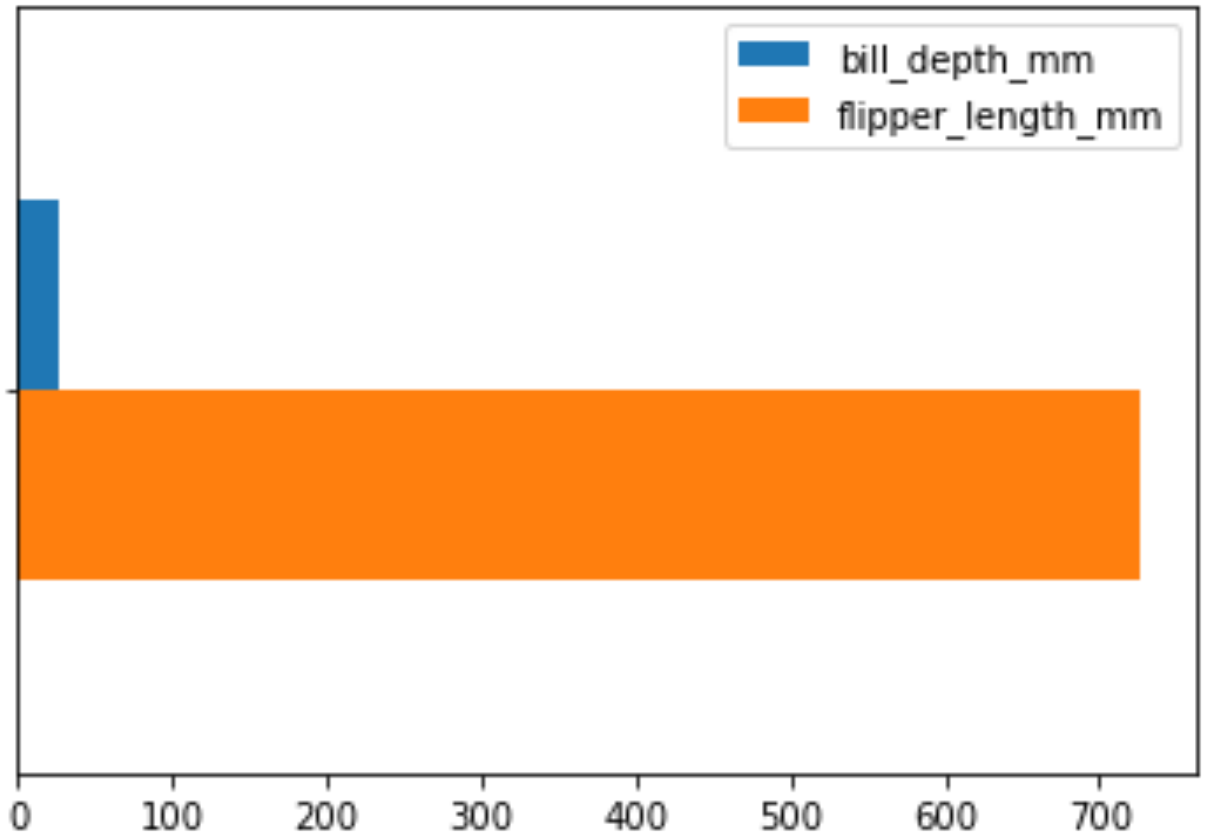
Linear Regression

*28*bill depth + 727*flipper length + 4199 = body mass*



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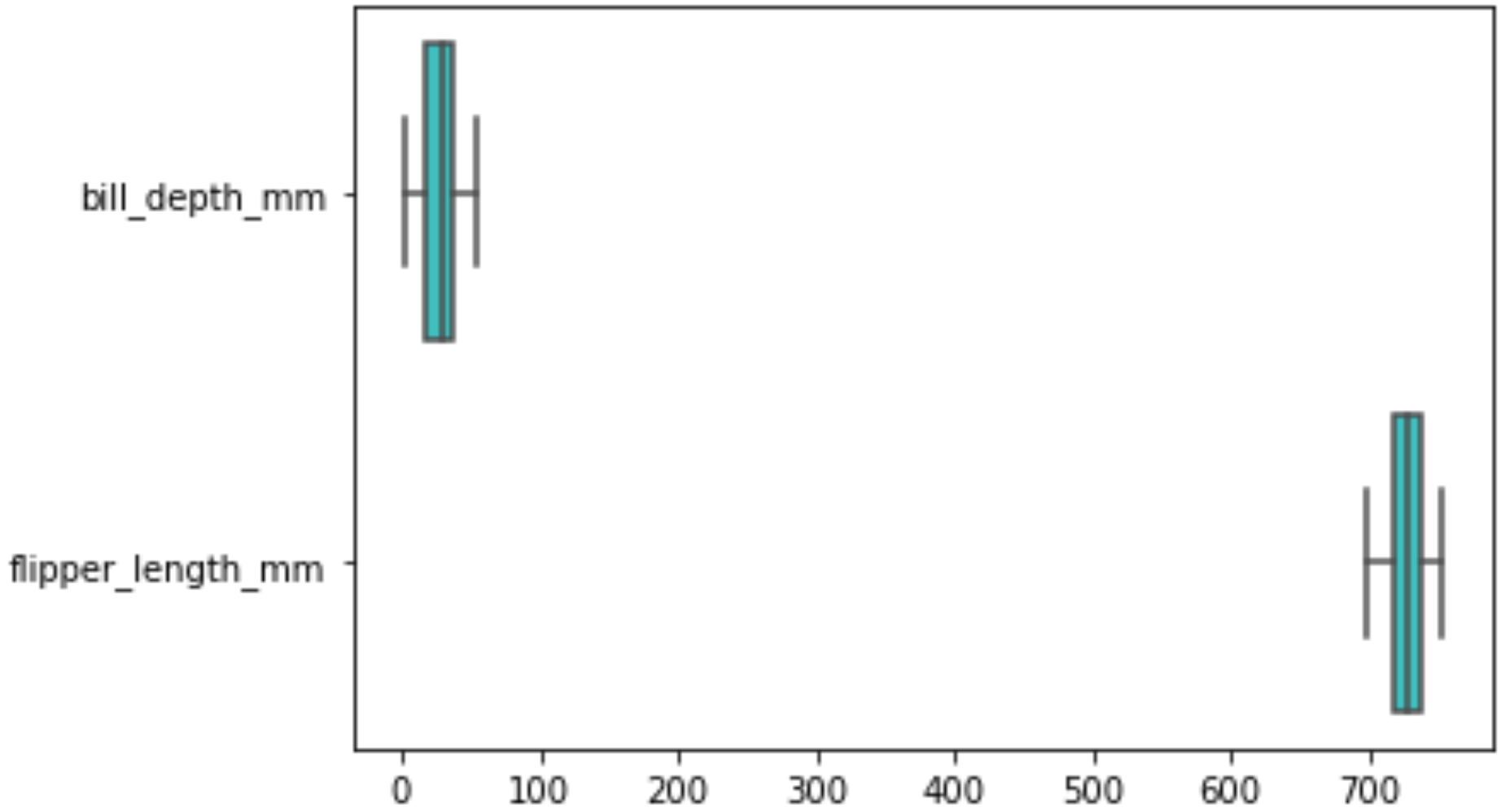
Linear Regression

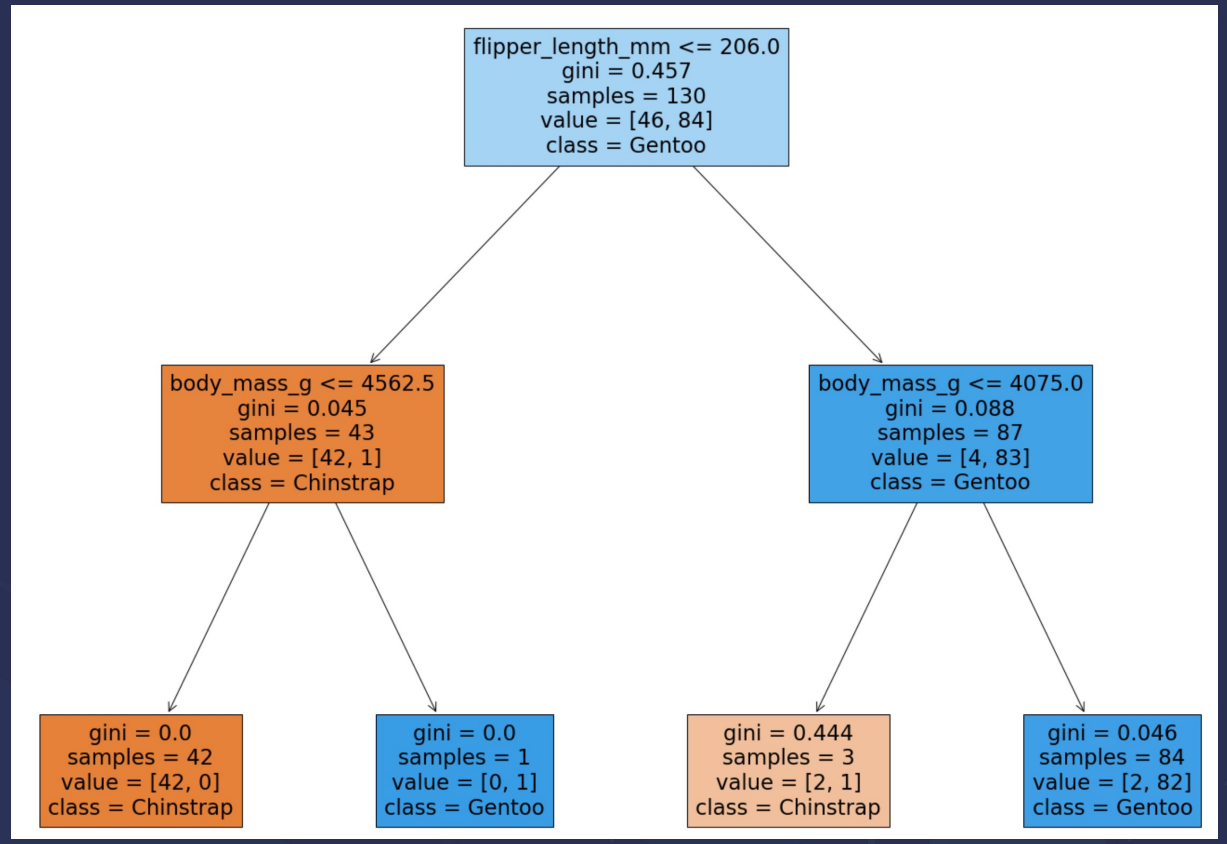


GO DATA DRIVEN

Decision Tree Classifer

GO DATA DRIVEN

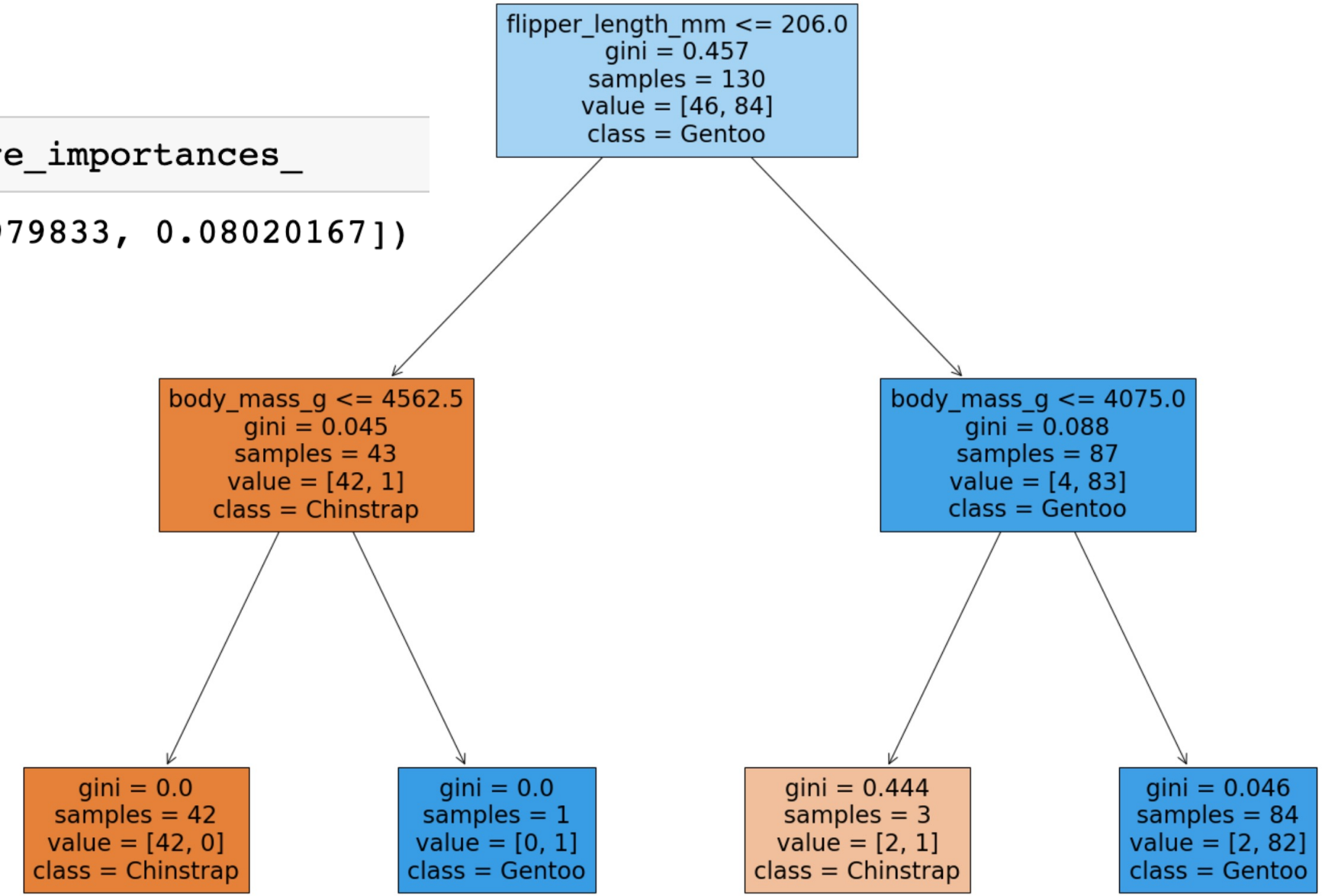
Global feature impotances



Decision Tree Classifier

```
model.feature_importances_
```

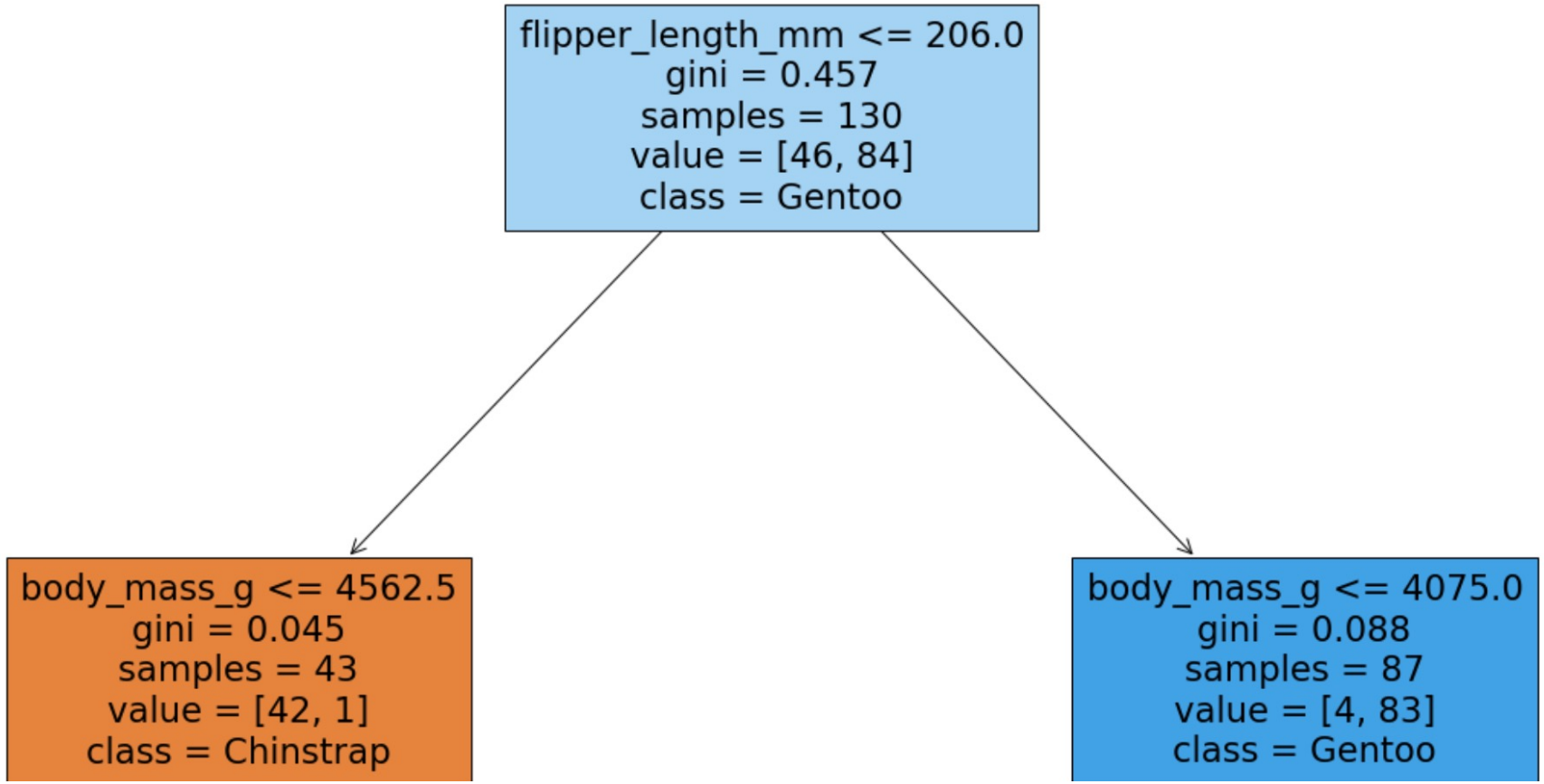
```
array([0.91979833, 0.08020167])
```



GO DATA DRIVEN

Decision Tree Classifier

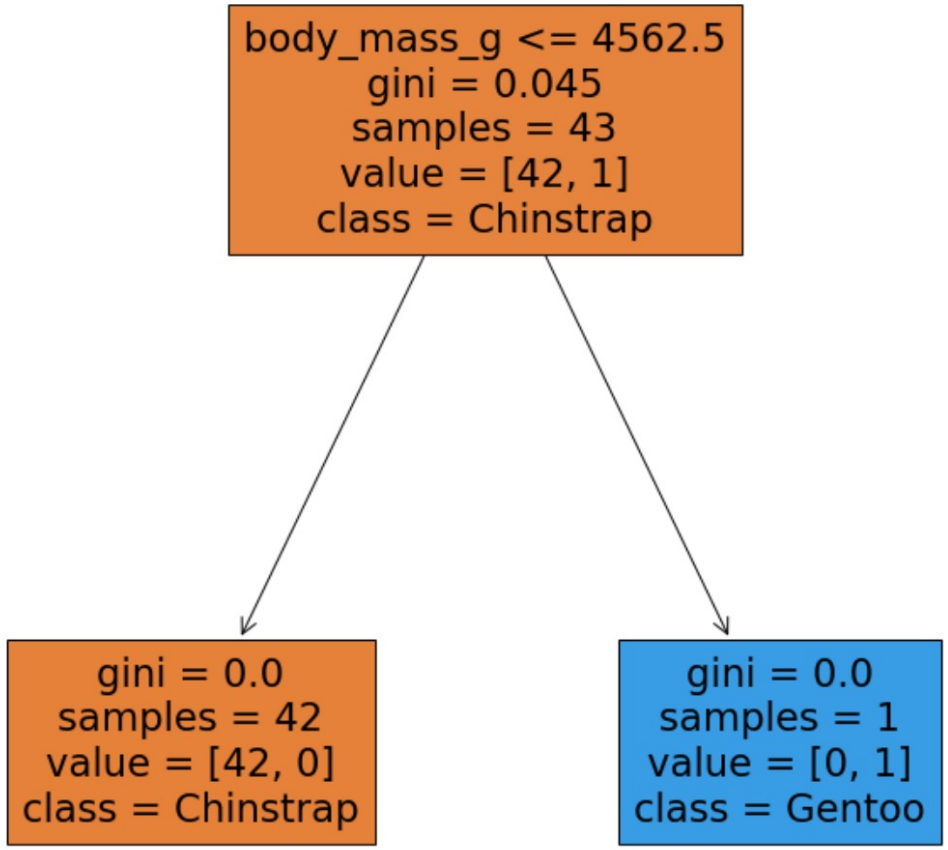
	feature importances
flipper_length_mm	0.919798
body_mass_g	0.080202

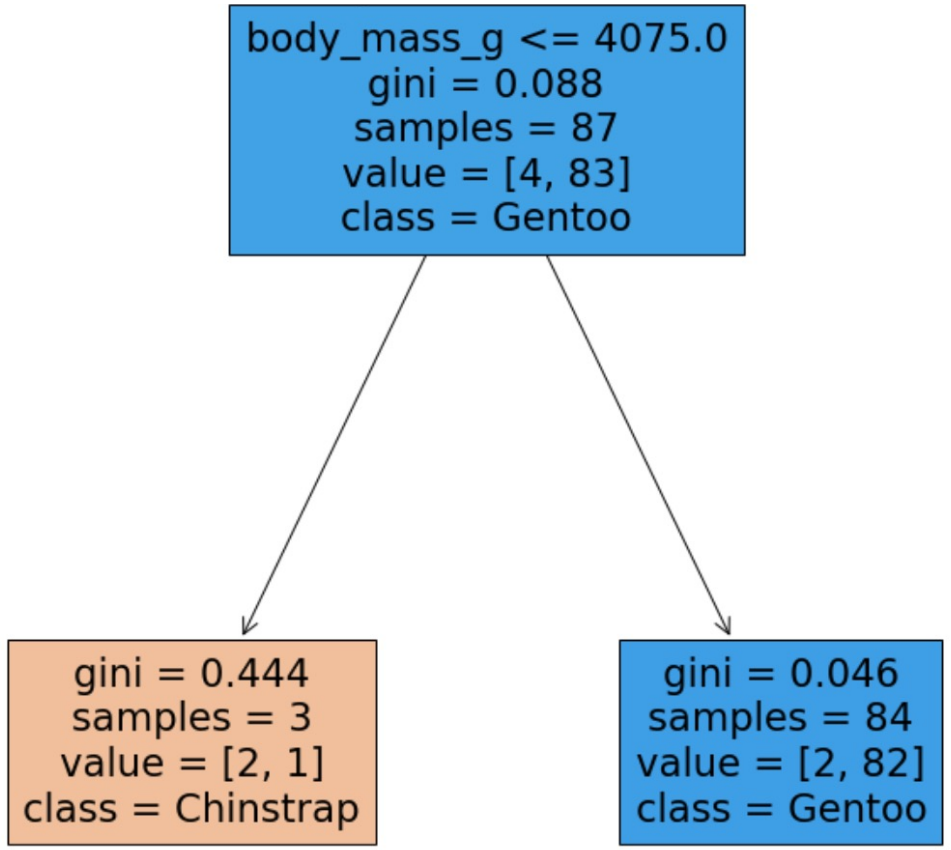


GO DATA DRIVEN

Decision Tree Classifier

feature importances	
flipper_length_mm	0.919798
body_mass_g	0.080202



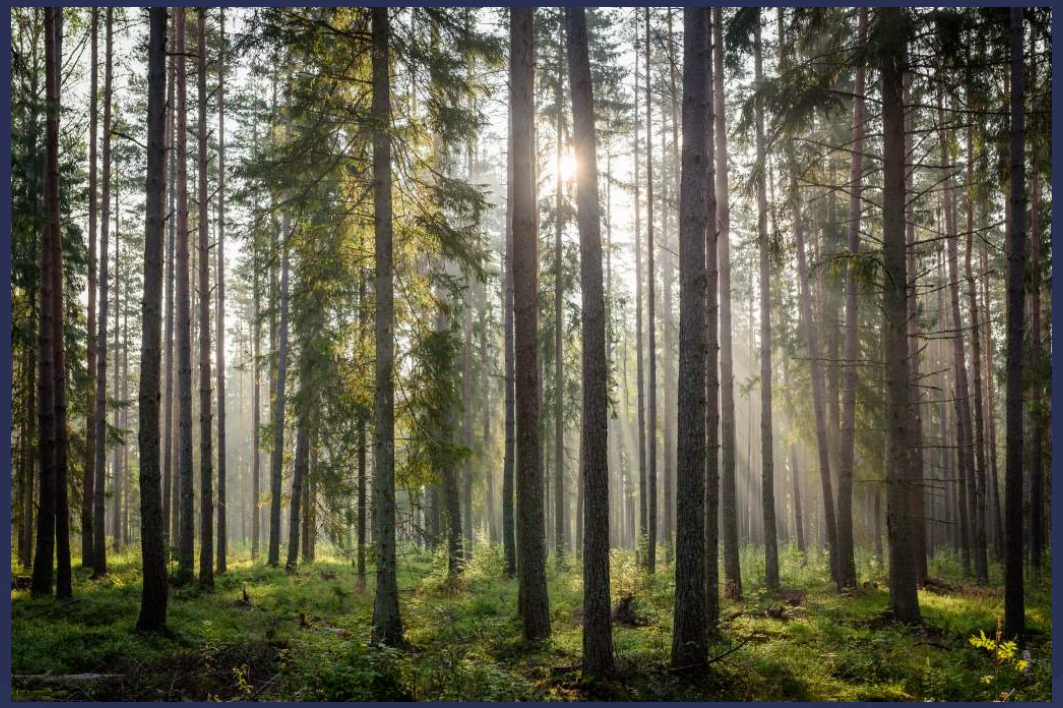


GO DATA DRIVEN

Random Forest Classifer

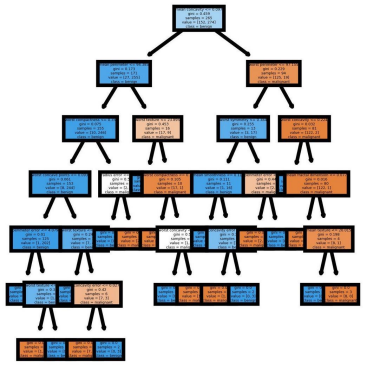
GO DATA DRIVEN

Global feature impotances

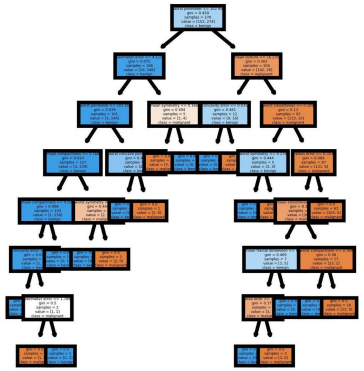


Random Forest Classifier

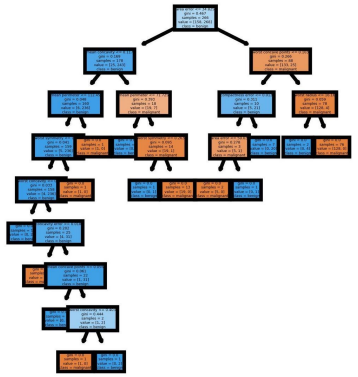
Estimator: 0



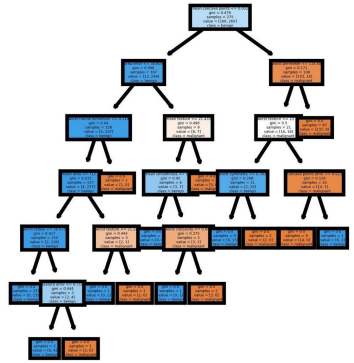
Estimator: 1



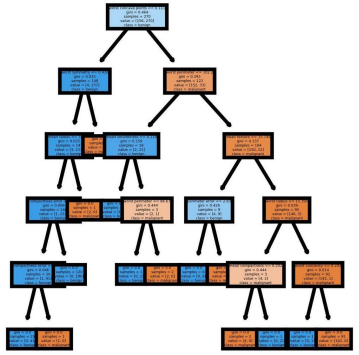
Estimator: 2



Estimator: 3



Estimator: 4

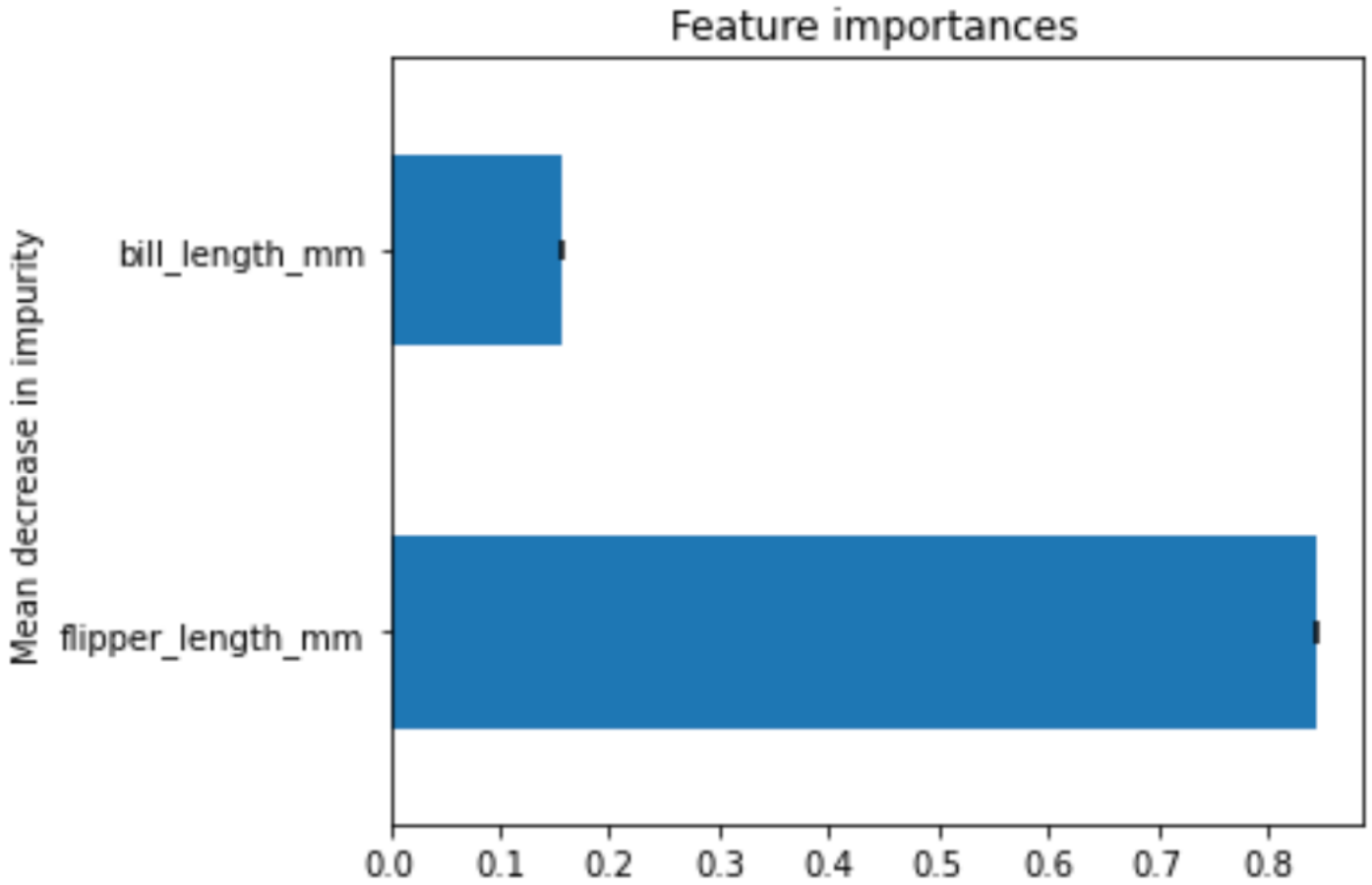


```
model.feature_importances_
```

```
array([0.84263378, 0.15736622])
```

GO DATA DRIVEN

Random Forest Classifier



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Jupyter Notebook 4

04_Permutation_Feature_Importance.ipynb

GO DATA DRIVEN

Model-Agnostic Feature Importance

	flipper_length_mm	bill_length_mm	bill_depth_mm	sex	island	species
27	187.0	40.5	17.9	Female	Biscoe	Adelie
292	221.0	48.2	15.6	Male	Biscoe	Gentoo
302	212.0	47.4	14.6	Female	Biscoe	Gentoo
62	185.0	37.6	17.0	Female	Biscoe	Adelie
181	205.0	52.8	20.0	Male	Dream	Chinstrap
15	185.0	36.6	17.8	Female	Torgersen	Adelie
231	216.0	49.0	16.1	Male	Biscoe	Gentoo
233	213.0	48.4	14.6	Male	Biscoe	Gentoo
87	189.0	36.9	18.6	Female	Dream	Adelie
159	197.0	51.3	18.2	Male	Dream	Chinstrap

0.856

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Drop Feature Importance

	flipper_length_mm	bill_length_mm	bill_depth_mm	sex	island	species
27	187.0	40.5	17.9	Female	Biscoe	Adelie
292	221.0	48.2	15.6	Male	Biscoe	Gentoo
302	212.0	47.4	14.6	Female	Biscoe	Gentoo
62	185.0	37.6	17.0	Female	Biscoe	Adelie
181	205.0	52.8	20.0	Male	Dream	Chinstrap
15	185.0	36.6	17.8	Female	Torgersen	Adelie
231	216.0	49.0	16.1	Male	Biscoe	Gentoo
233	213.0	48.4	14.6	Male	Biscoe	Gentoo
87	189.0	36.9	18.6	Female	Dream	Adelie
159	197.0	51.3	18.2	Male	Dream	Chinstrap

0.856

	flipper_length_mm	bill_length_mm	sex	island	species
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292	221.0	48.2	Male	Biscoe	Gentoo
302	212.0	47.4	Female	Biscoe	Gentoo
62	185.0	37.6	Female	Biscoe	Adelie
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231	216.0	49.0	Male	Biscoe	Gentoo
233	213.0	48.4	Male	Biscoe	Gentoo
87	189.0	36.9	Female	Dream	Adelie
159	197.0	51.3	Male	Dream	Chinstrap

???

GO DATA DRIVEN

Permutation Feature Importance

	flipper_length_mm	bill_length_mm	bill_depth_mm	sex	island	species
27	187.0	40.5	17.9	Female	Biscoe	Adelie
292	221.0	48.2	15.6	Male	Biscoe	Gentoo
302	212.0	47.4	14.6	Female	Biscoe	Gentoo
62	185.0	37.6	17.0	Female	Biscoe	Adelie
181	205.0	52.8	20.0	Male	Dream	Chinstrap
15	185.0	36.6	17.8	Female	Torgersen	Adelie
231	216.0	49.0	16.1	Male	Biscoe	Gentoo
233	213.0	48.4	14.6	Male	Biscoe	Gentoo
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0.856

	flipper_length_mm	bill_length_mm	sex	island	species
27	187.0	40.5	Female	Biscoe	Adelie
292	221.0	48.2	Male	Biscoe	Gentoo
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233	213.0	48.4	Male	Biscoe	Gentoo
87	189.0	36.9	Female	Dream	Adelie
159	197.0	51.3	Male	Dream	Chinstrap

???

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Permutation Feature Importance

Advantages

- Works on a **global** level for a model
- Displays a feature's **importance**
- **Fast** to calculate
- **Additional** tricks

Disadvantages

- Dependent on **randomness**
- Misleading for **correlations**
- Can lead to **unrealistic data** points
- Need access to **true** outcome
- Does not tell you how **sensitive** a model is to a feature

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Jupyter Notebook 5

05_Partial_Dependence_Plots.ipynb

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Global Sensitivity

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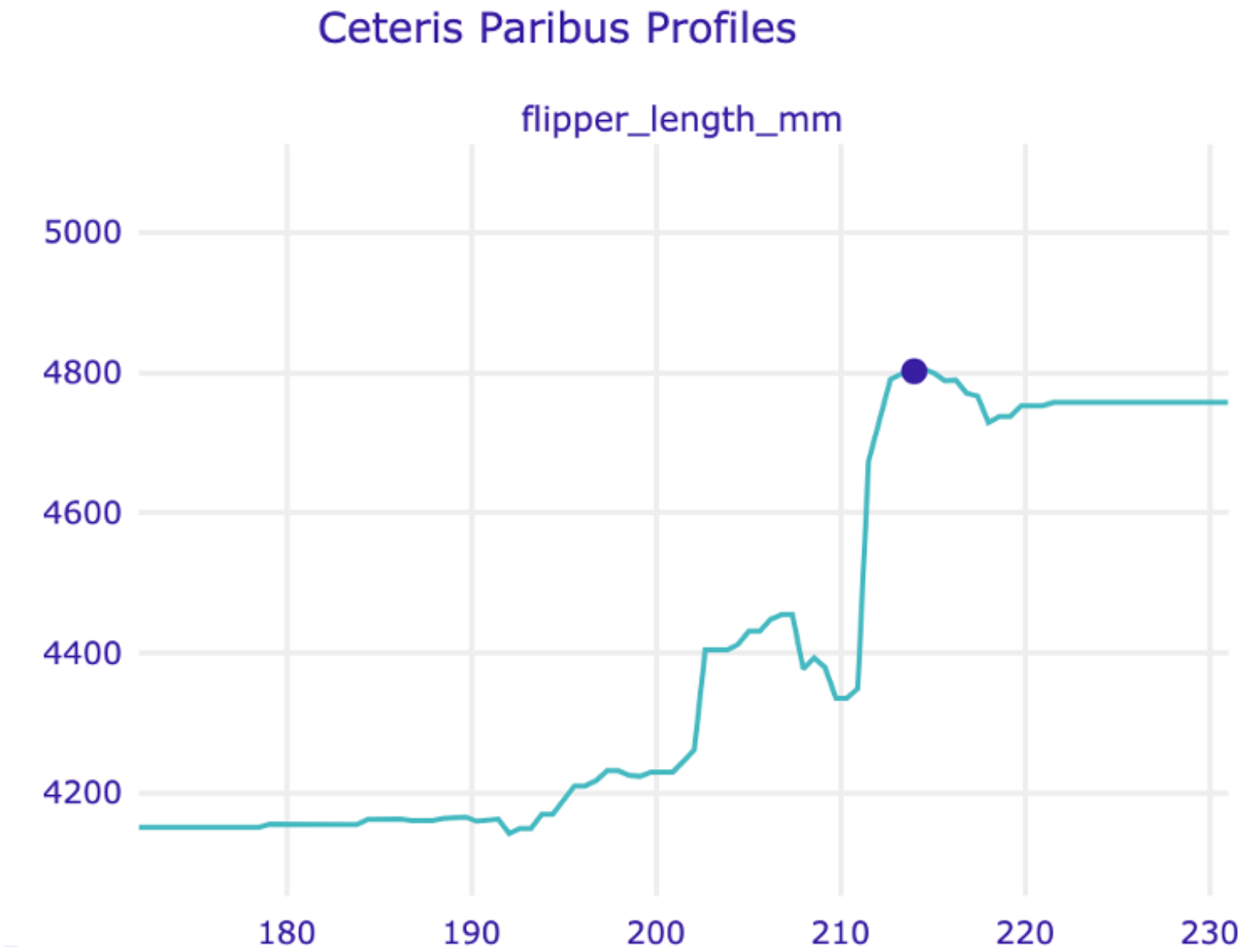
Ceteris Paribus

- **Sensivity** to feature
- On a **local** level



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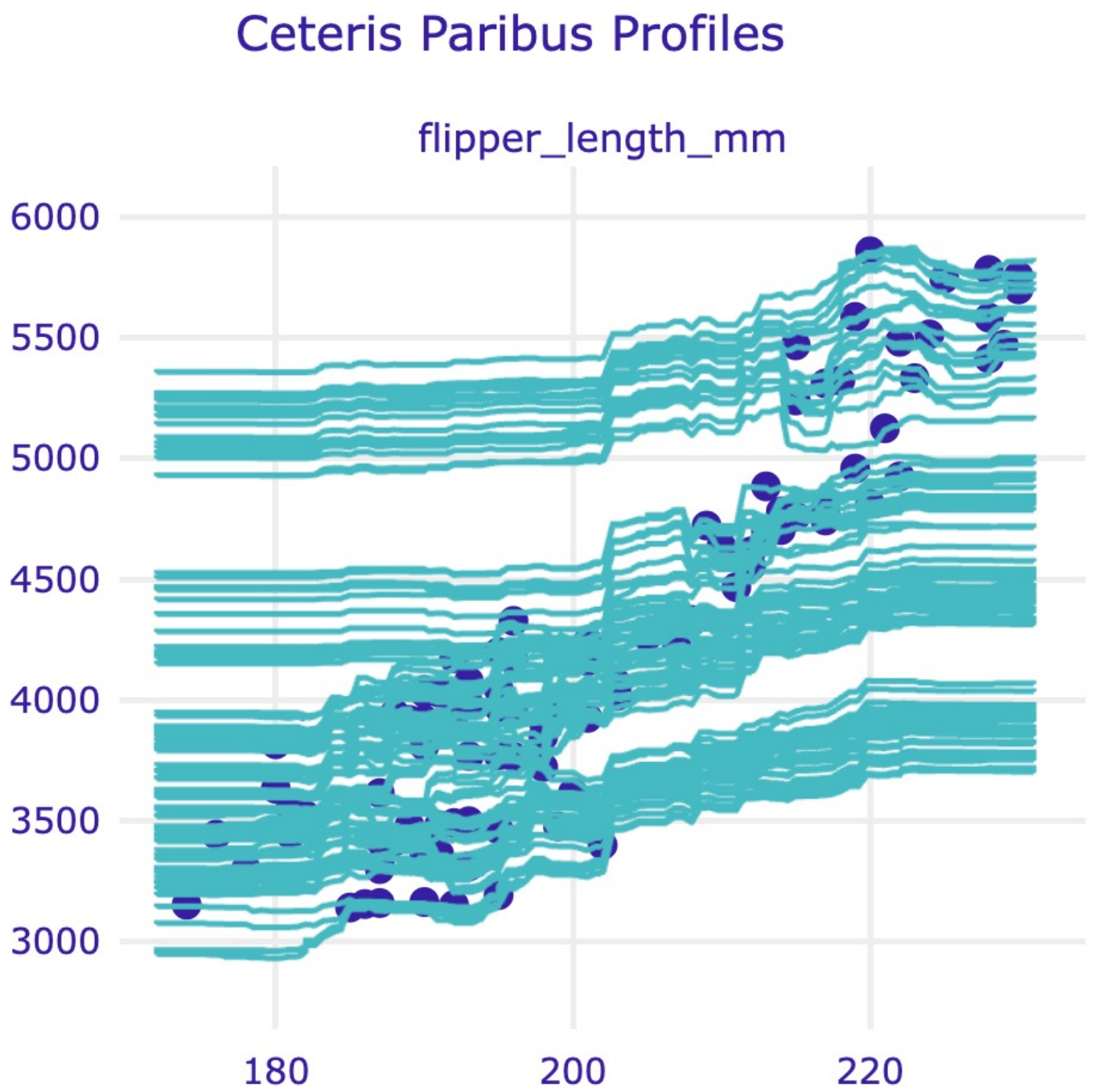
Individual Conditional Expectation

- **Sensivity** to feature
- One line per instance



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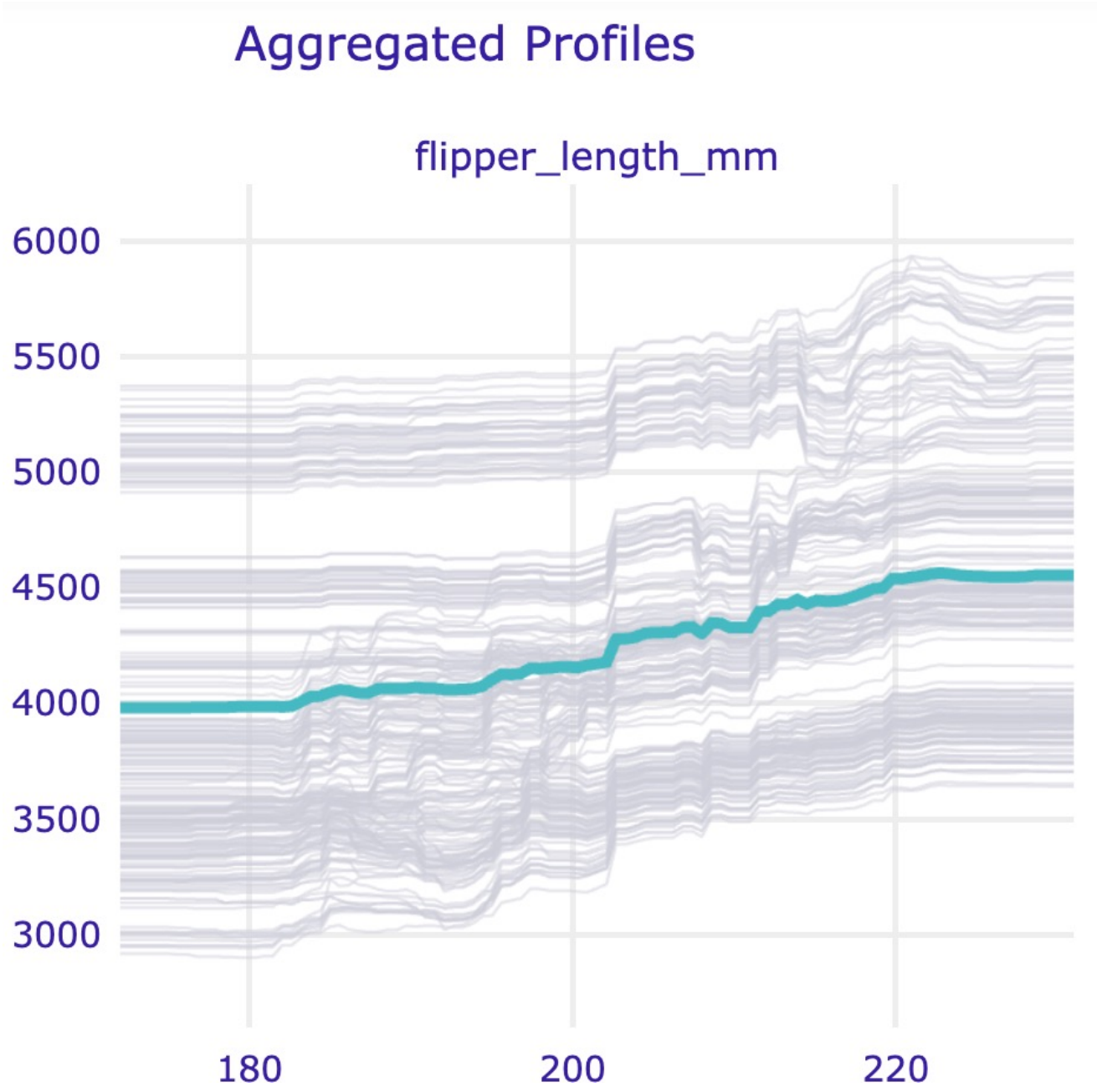
Partial Dependence Plot

- **Sensivity** to feature
- Average of ICE plot
- **Global method**



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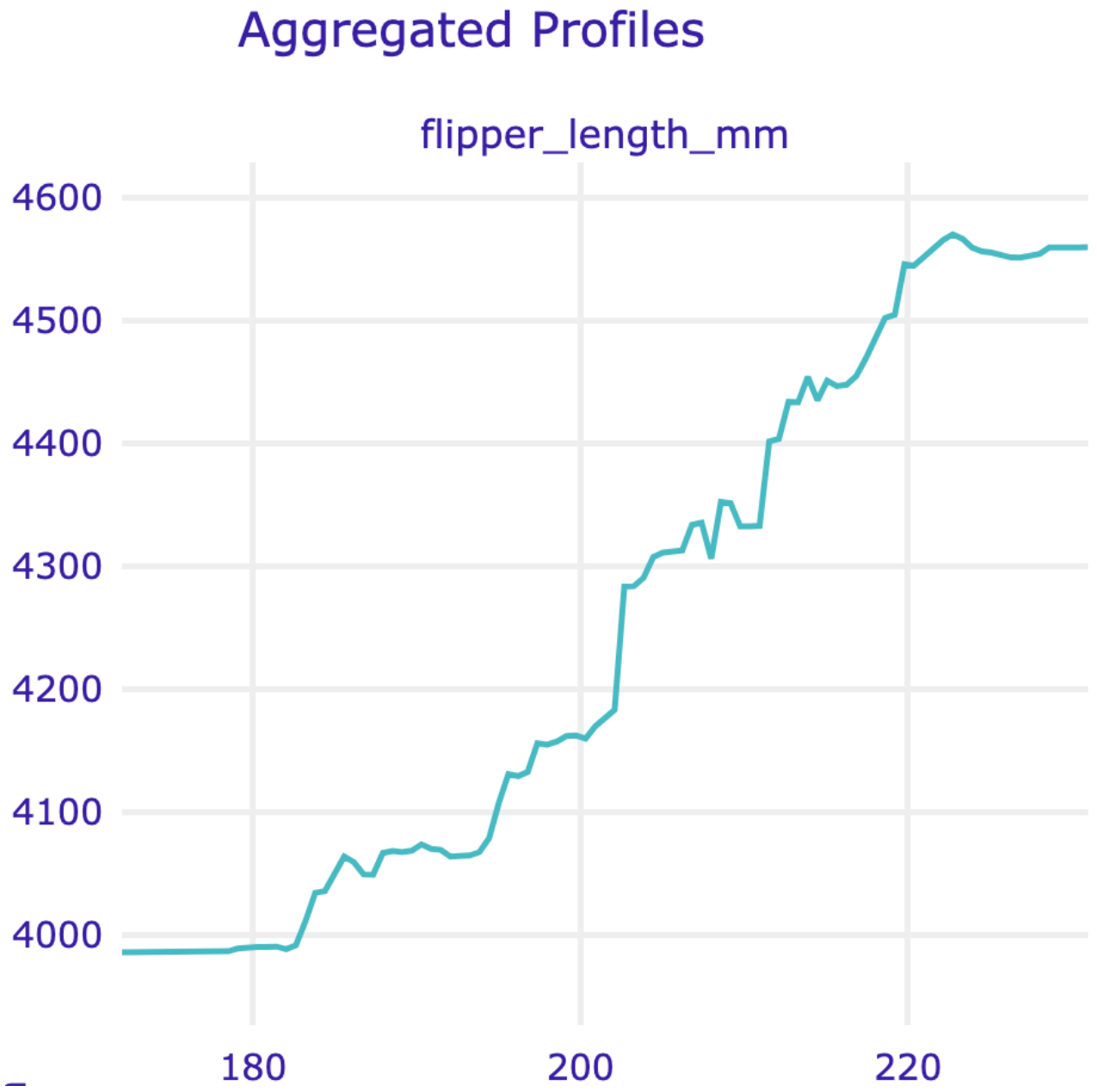
Partial Dependence Plot

- **Sensivity** to feature
- Average of ICE plot
- **Global method**



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Summary

- Intrinsicly interpretable machine learning models
- Model-agnostic interpretability techniques

	Local	Global
Importance	Break-down plots	Permutation Feature Importance
Sensivitiy	Ceteris Paribus	Partial Dependence Plots

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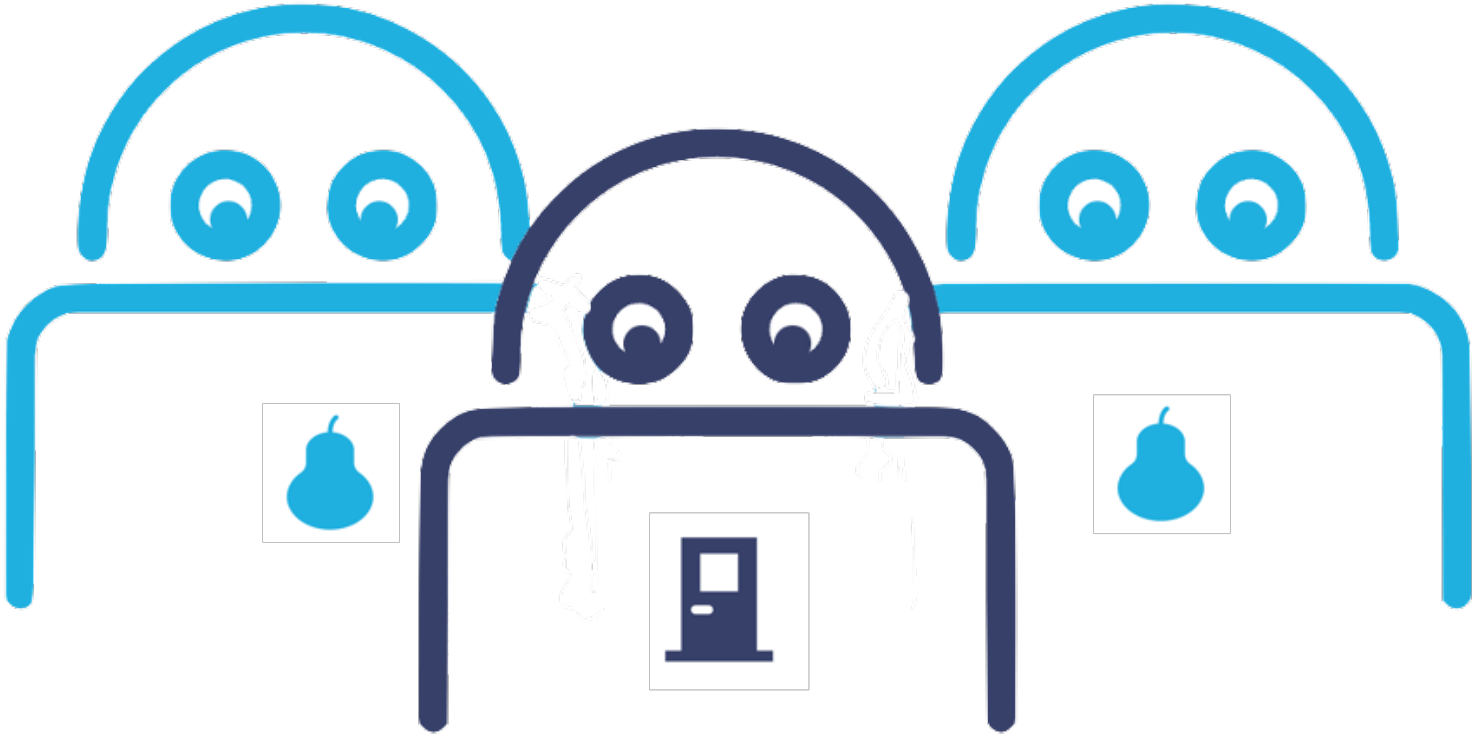
Hackathon!

- Credit Lending
- Laptop Prices
- Medical Diagnoses
- Discussion Hackathon (theory)



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Unpacking the Black Box

How to Interpret your Machine Learning Model

GoDataDriven

@ AMLD Switzerland 2022

The Data & AI Maturity Journey

13:30-17:30, March 28 @ 1A

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Unpacking the Black Box

How to Interpret your Machine Learning Model