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TEXAS
The University of Texas at Austin

Python for Data Science

Overview, Workflows, and Exercises

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HPC Applications

Data Science Overview

Data science is used to drive decision making under **uncertainty**

Python is a key part of the data science toolbox

Data Science / Machine Learning / Statistics

Statistics: applied mathematics to **describe data** in terms of probability

- How does this system work?
- What is the probability of either my observed data or my hypothesis?

Machine Learning: applied statistics to **predict outcomes**

- What variables are good predictors of the outcome of interest?
- How does adding new data improve prediction?

Data Science: combine statistics, machine learning, and **domain expertise** to drive decision making.

Python for Data Science Requirements

Python experience

- you know what **variables** are and how to assign them
- you're familiar with basic **data types** (floats, integers, strings)

Data experience

- you've worked with **spreadsheets** before
- you're comfortable reading **graphs** like scatter plots or histograms

Statistics experience

- you're familiar with **descriptive statistics** (mean, standard deviation, etc.)
- you've seen linear **regression** before

Statistical Models for Data

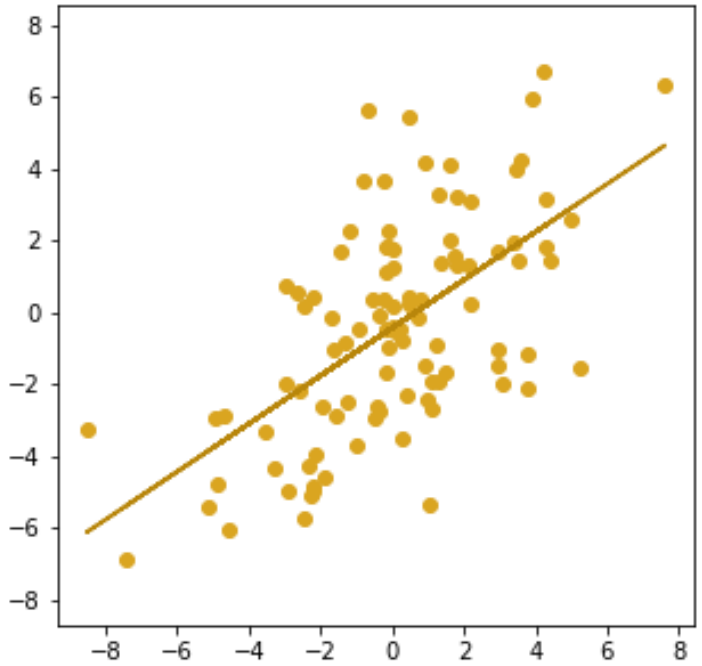
Classification

Iris setosa

Iris virginica

Iris versicolor

Regression



Statistical Models for Data

Classification	Regression
Logistic regression	Linear regression (many types)
Multinomial regression	Random forest
Decision tree	
Random forest	
Support vector machine	
Clustering	

Machine Learning Models for Data

Supervised

Labeled data / known outcomes

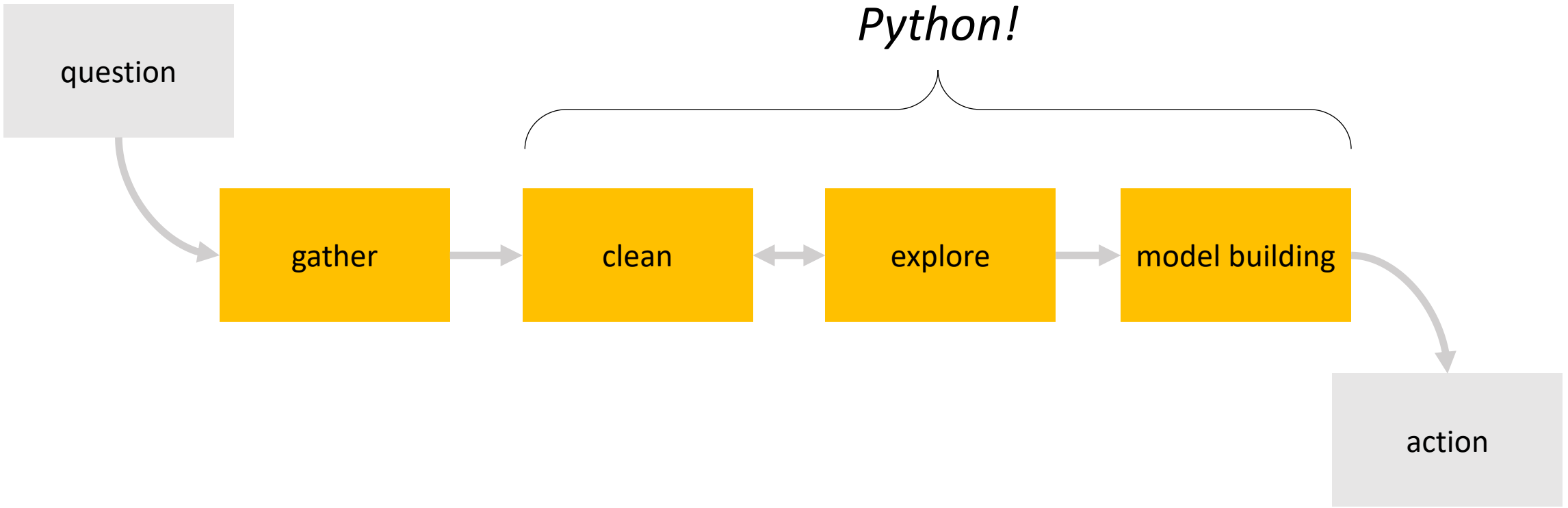
Learn a data **model**

Unsupervised

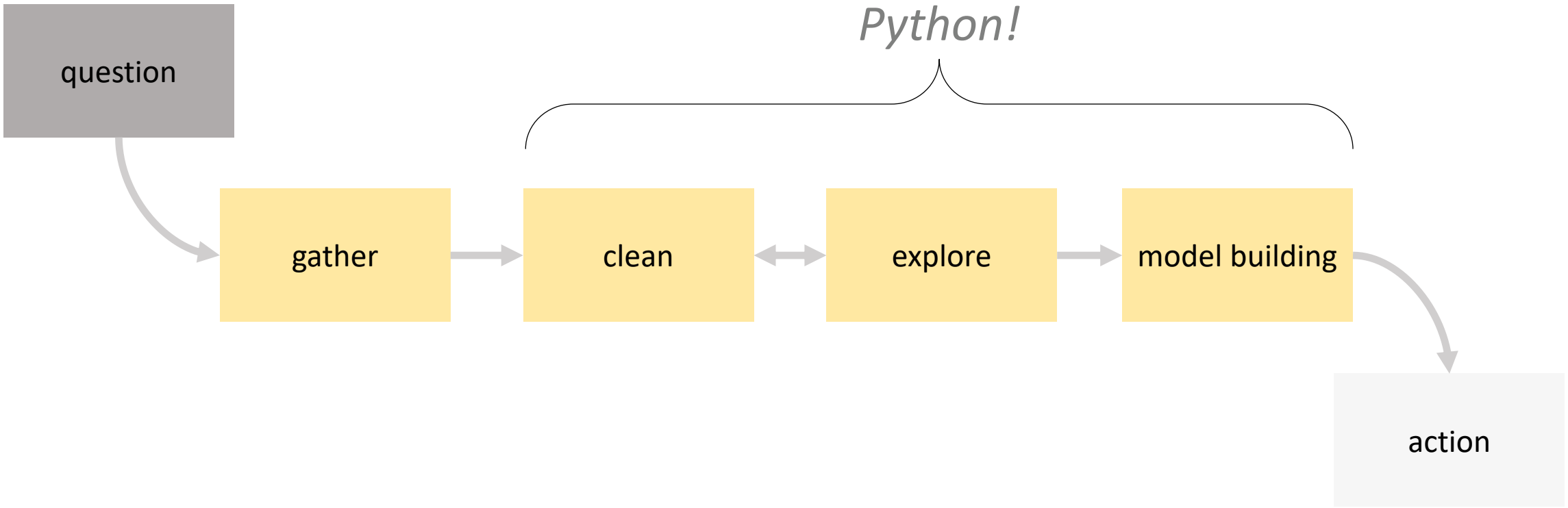
Unlabeled data / unknown outcomes

Learn data **structure**

Data science workflow



Data science workflow



Question: Can we classify plant species?

Iris setosa

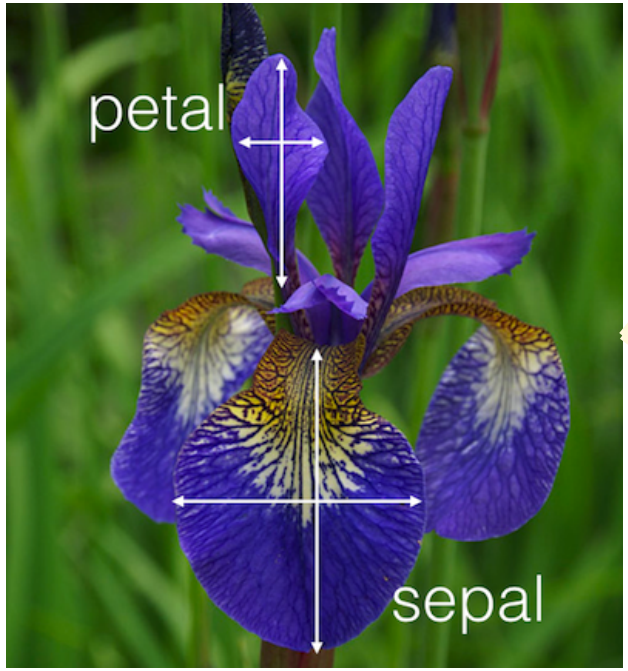
Iris versicolor

Iris virginica

https://en.wikipedia.org/wiki/Iris_flower_data_set

Question: Can we classify plant species?

Can we identify species of iris by their petal and sepal lengths and widths?



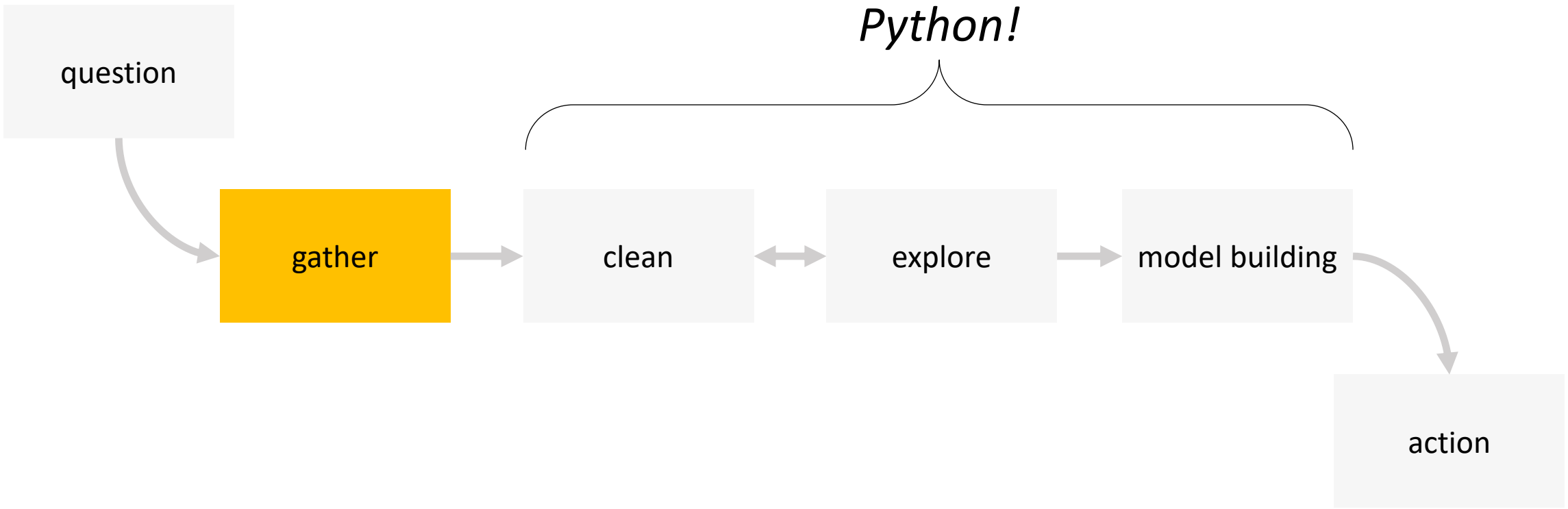
Iris setosa

Iris virginica

Iris versicolor

https://observablehq.com/@sandroormeno/tensorflow-con-iris

Data science workflow



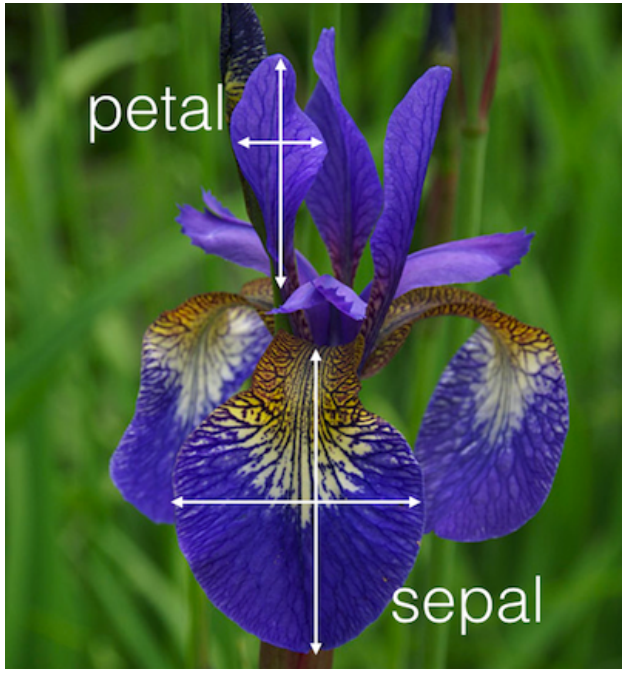
Gather Data: The *Iris* dataset

Morphological data on three *Iris* species

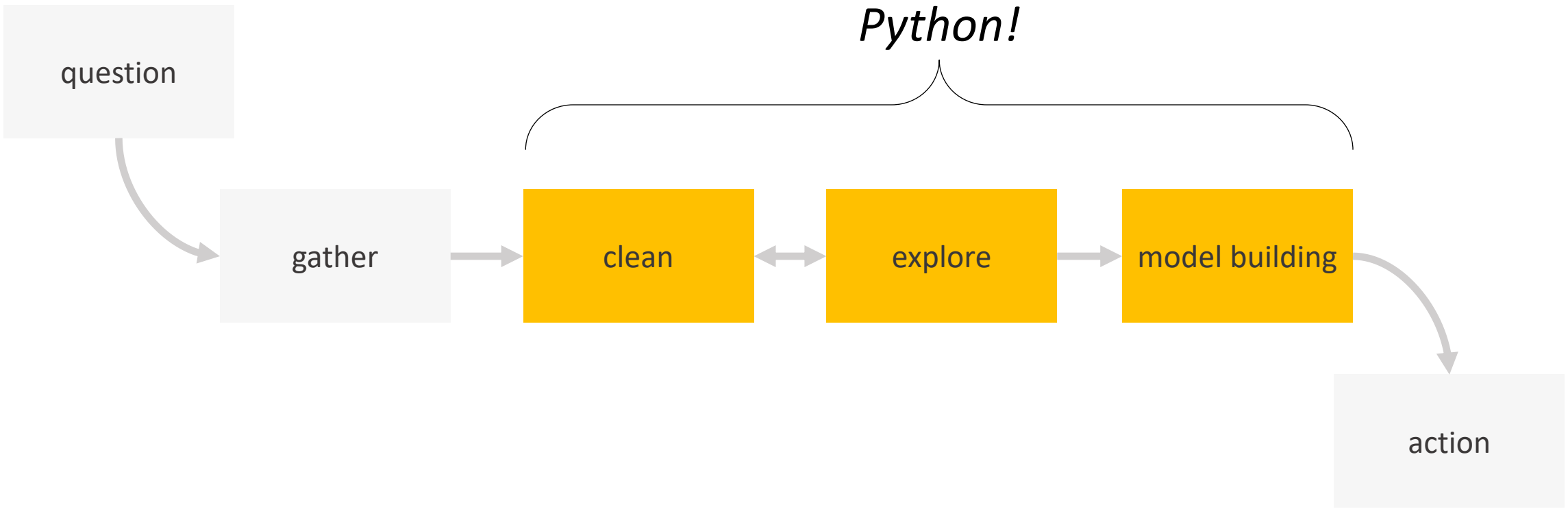
Collected by Edgar Anderson; introduced by RA Fisher in 1936

Extensively used in statistics and machine learning training

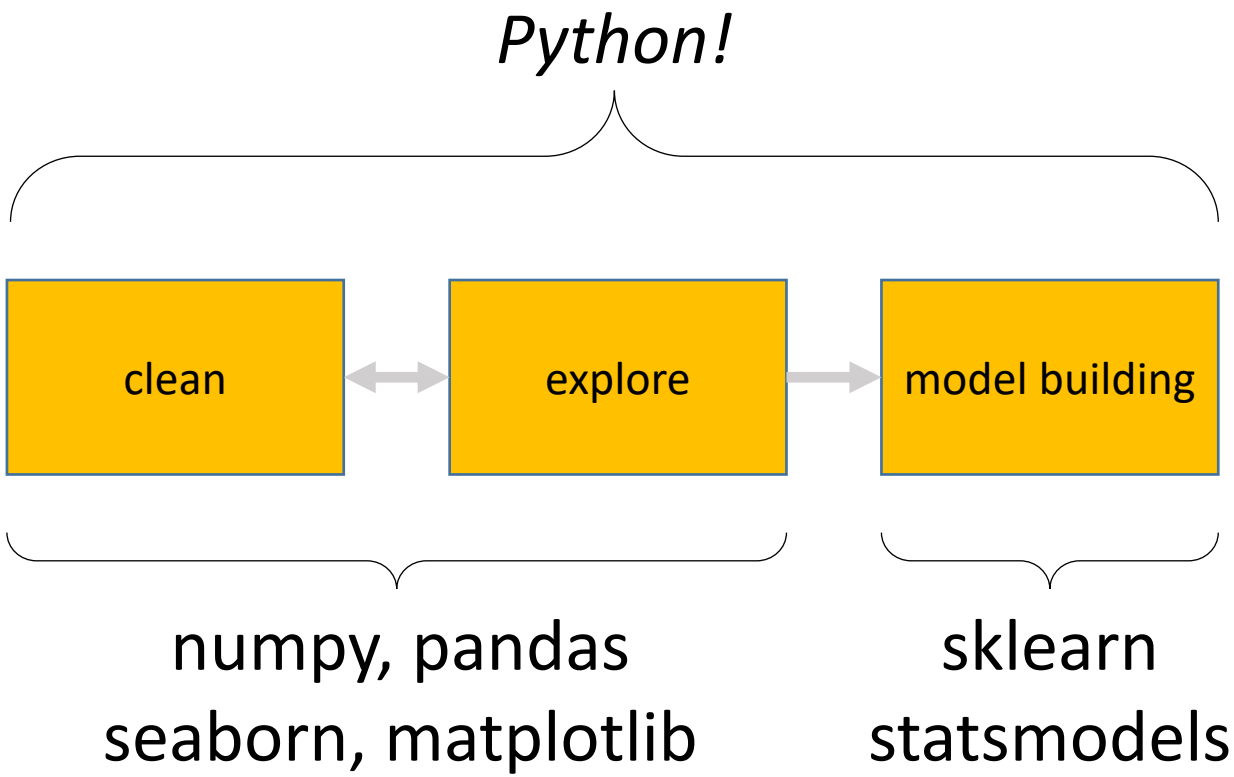
Distributed with sklearn and other libraries



Data science workflow



Python's Data Science Stack



Clean data are easier to analyze

Format data in a way Python can read

- **“.csv” or “.txt” files are easiest to work with**
- Some libraries, like pandas, can handle “.xls” or “.xlsx” files
- Excel, Numbers, etc. can export data to “.csv” or “.txt”

Organized data are easier to analyze

Use **long** format instead of **wide** format when possible

Long format data have one observation per row:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

Organized data are easier to analyze

Use **long** format instead of **wide** format when possible

Wide format data have multiple observations per row:

	sepal length (cm)			sepal width (cm)			petal length (cm)			petal width (cm)		
species	setosa	versicolor	virginica	setosa	versicolor	virginica	setosa	versicolor	virginica	setosa	versicolor	virginica
0	5.1	NaN	NaN	3.5	NaN	NaN	1.4	NaN	NaN	0.2	NaN	NaN
1	4.9	NaN	NaN	3.0	NaN	NaN	1.4	NaN	NaN	0.2	NaN	NaN
2	4.7	NaN	NaN	3.2	NaN	NaN	1.3	NaN	NaN	0.2	NaN	NaN
3	4.6	NaN	NaN	3.1	NaN	NaN	1.5	NaN	NaN	0.2	NaN	NaN
4	5.0	NaN	NaN	3.6	NaN	NaN	1.4	NaN	NaN	0.2	NaN	NaN

Organized data are easier to analyze

Use **long** format instead of **wide** format when possible

Python can convert your data between these two formats:

- Pandas “**melt**” converts wide -> long
- Pandas “**pivot**” or “**pivot_table**” convert long -> wide

Cat behavior data (conceptual example)

This is Twinky. She likes
- Sitting in the bathroom sink
- Meowing loudly

This is Columbo. He likes
- Snuggling
- Chasing toys

Cat behavior data, wide format

Name	Date	Time	Location_1	Date	Time	Location_2
Twinky	1/1/19	1:00p	sunny spot in chair	1/1/19	3:00p	food dish
Columbo	1/1/19	1:15p	cat bed	1/1/19	2:30p	litter box

Cat behavior data, **long** format

Name	Date	Time	Location
Twinky	1/1/19	1:00p	sunny spot in chair
Twinky	1/1/19	3:00p	food dish
Columbo	1/1/19	1:15p	cat bed
Columbo	1/1/19	2:30p	litter box

Data cleaning also involves:

Checking for **type consistency**

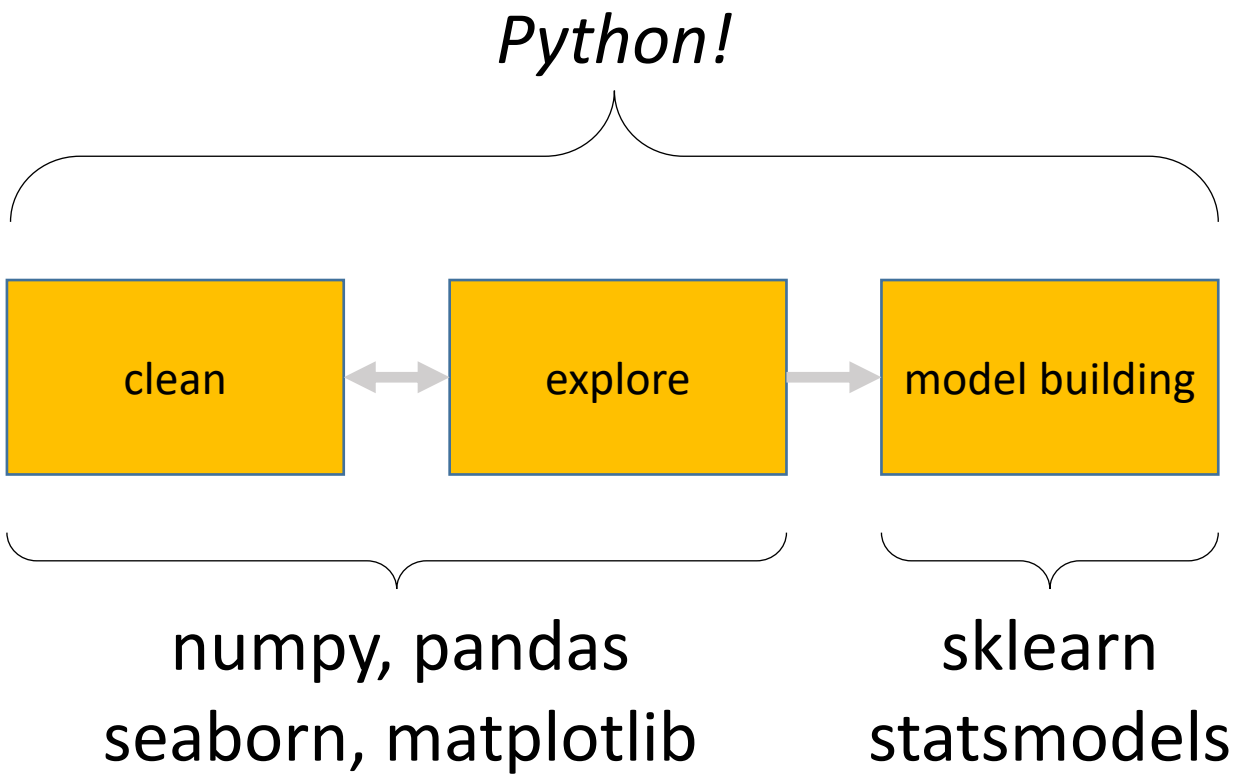
- Numbers where you expect numbers
- Characters where you expect characters

Looking for **missing data**, and determining how to handle it

Removing contaminating data (e.g. spaces or special characters) from your dataset

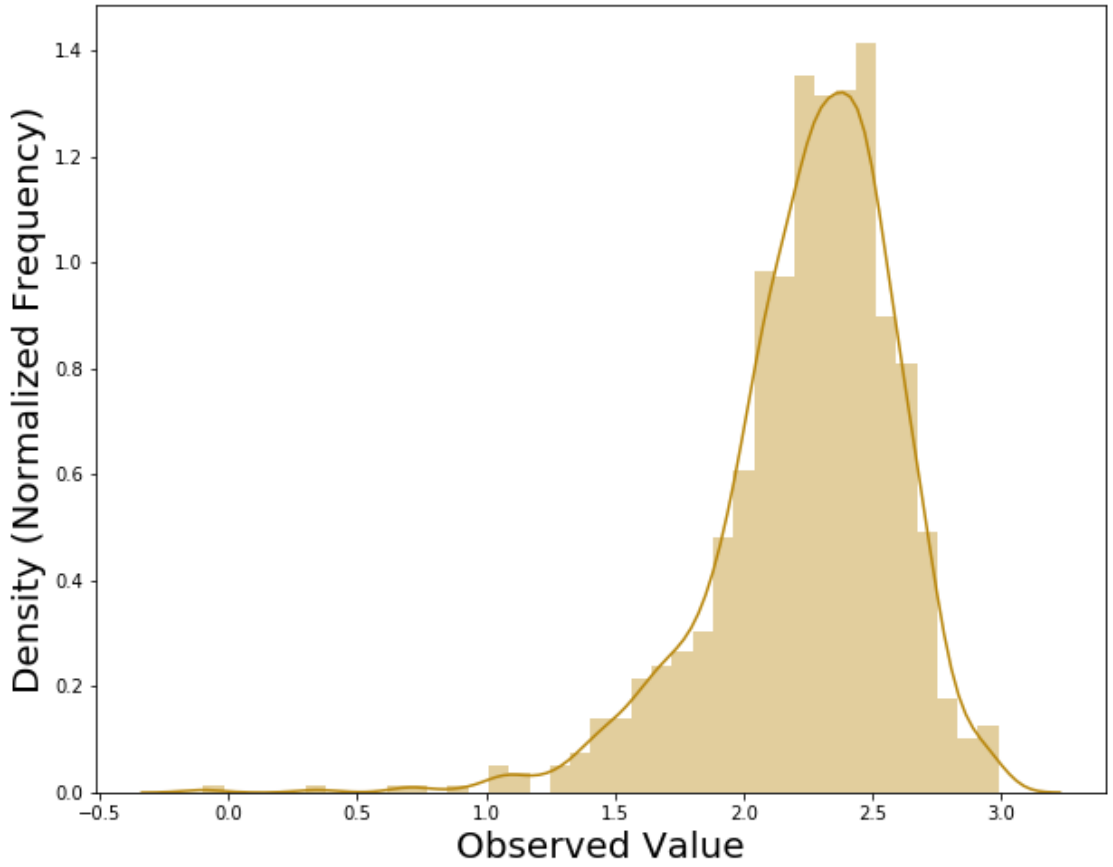
We'll explore some ways of doing this in Python in the hands-on exercise.

Exploring Data with Python's Science Stack



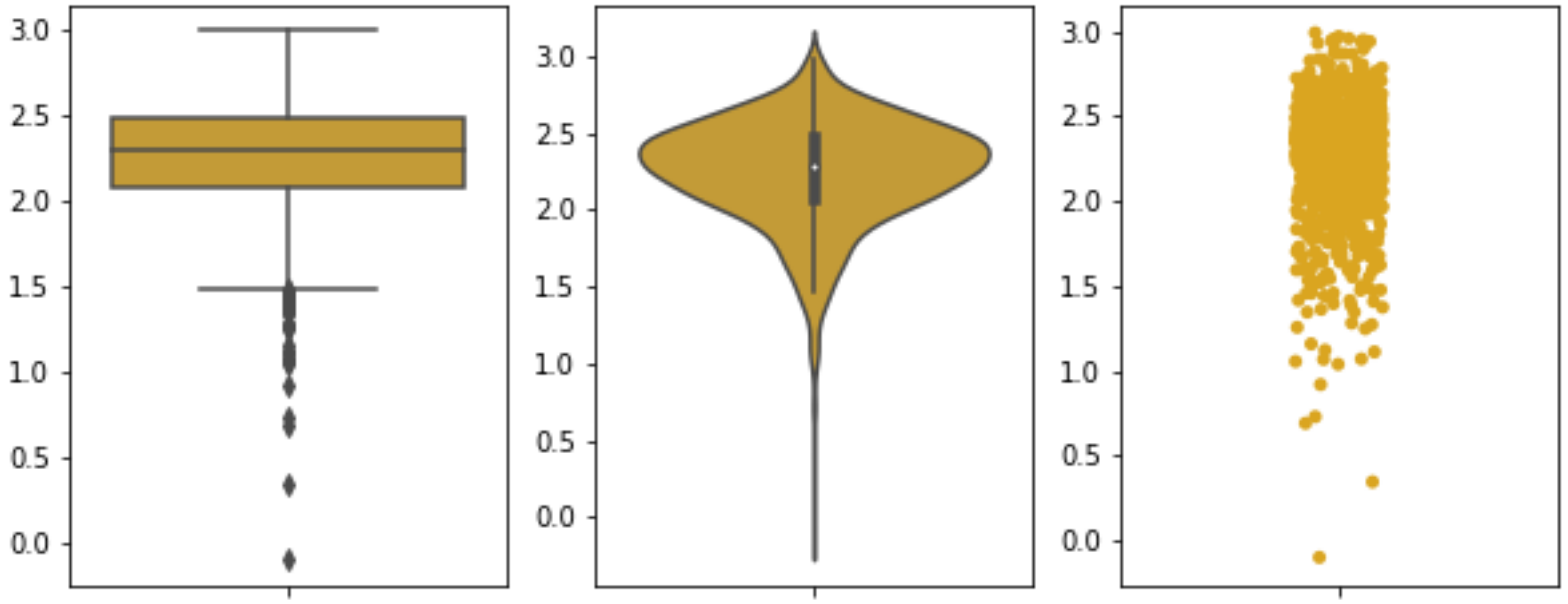
Exploring Data through Visualization

Histograms show the frequency of observations of a single value



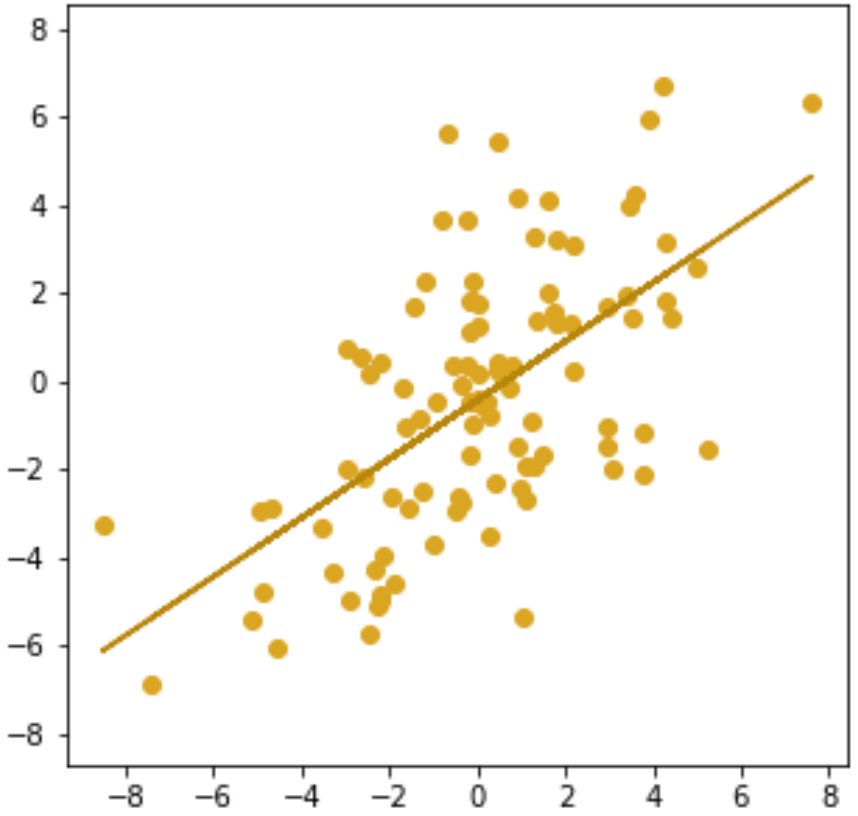
Exploring Data through Visualization

Boxplots, violin plots, and **strip plots** also show data distributions



Exploring Data through Visualization

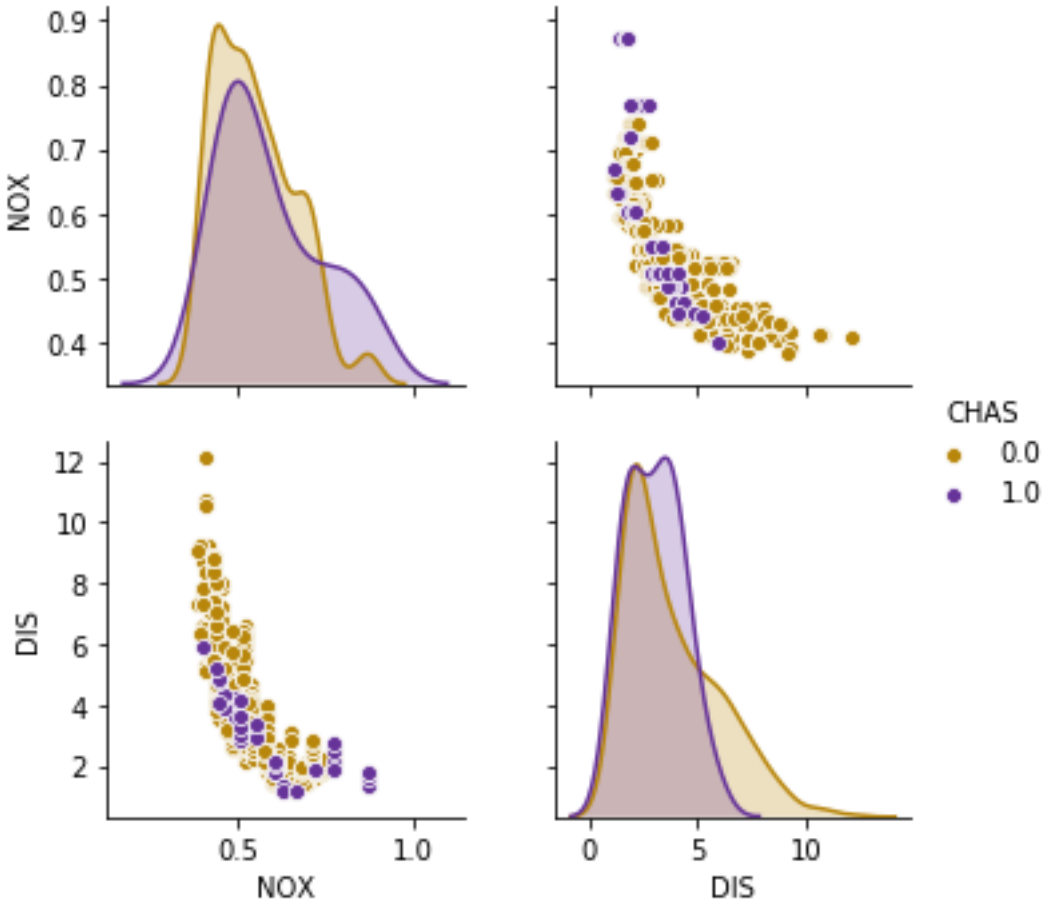
Scatterplots show the correlation between two variables



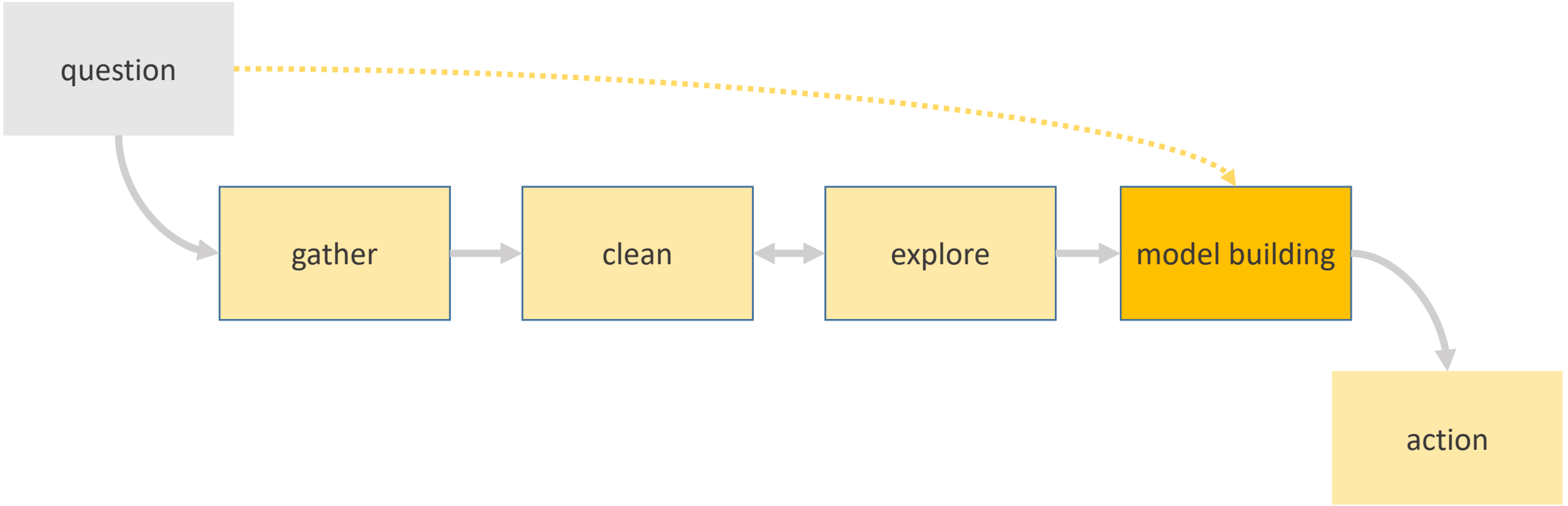
Exploring Data through Visualization

Pair plots make scatterplots for each pair of variables in a dataset, and histograms for each variable.

They can also be colored by categorical variables.

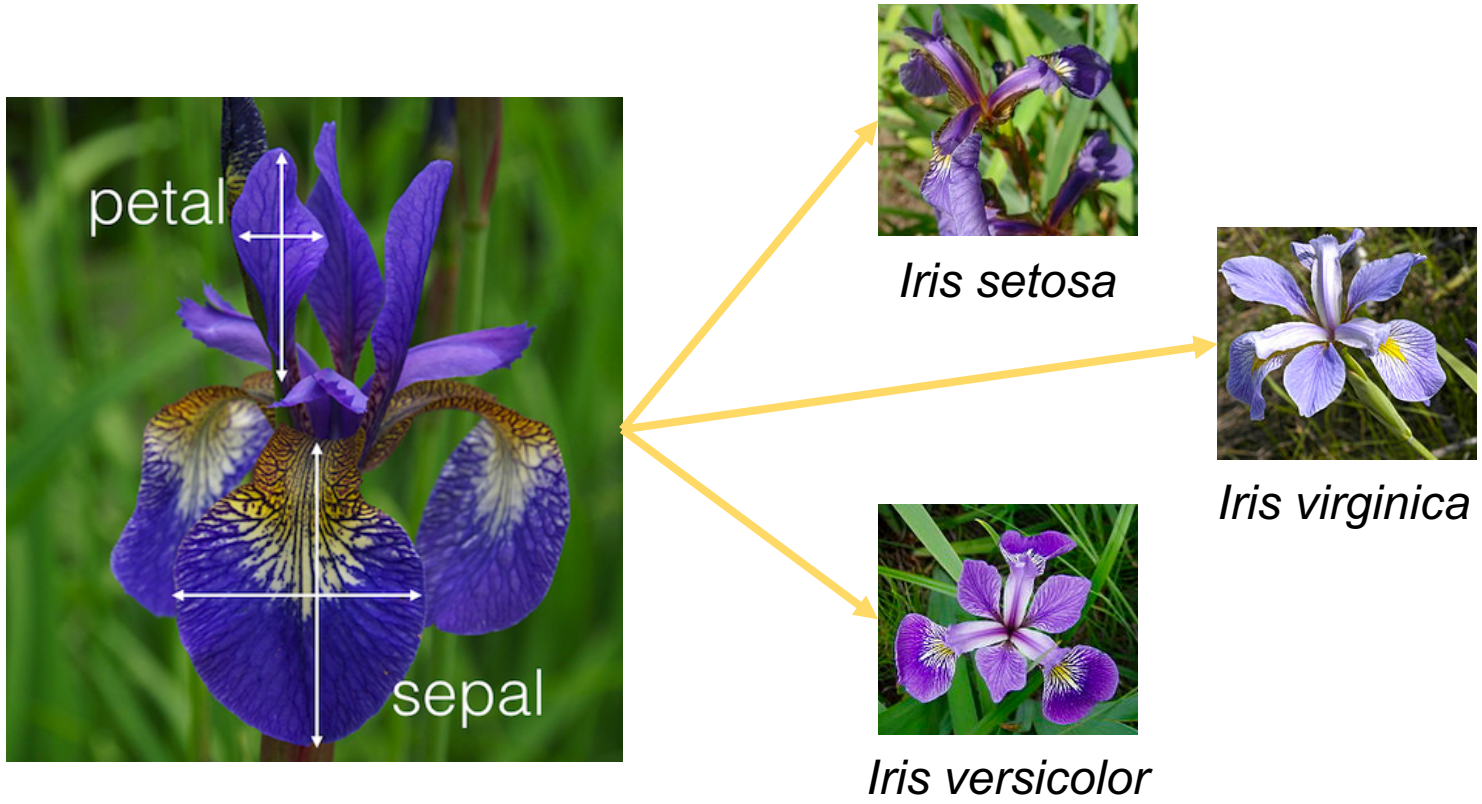


Model Building



Model Selection: Plant classification

Our example is a **supervised classification** problem: we want to group observations by a category (species), and we have labeled training data.



https://observablehq.com/@sandroormeno/tensorflow-con-iris

Model Training and Testing

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4	5.0	3.6	1.4	0.2	setosa

Most of the data (70-80%) are used for model **training**.

The remainder are set aside (not used), and reserved for **testing** the model.

Model Training and Testing

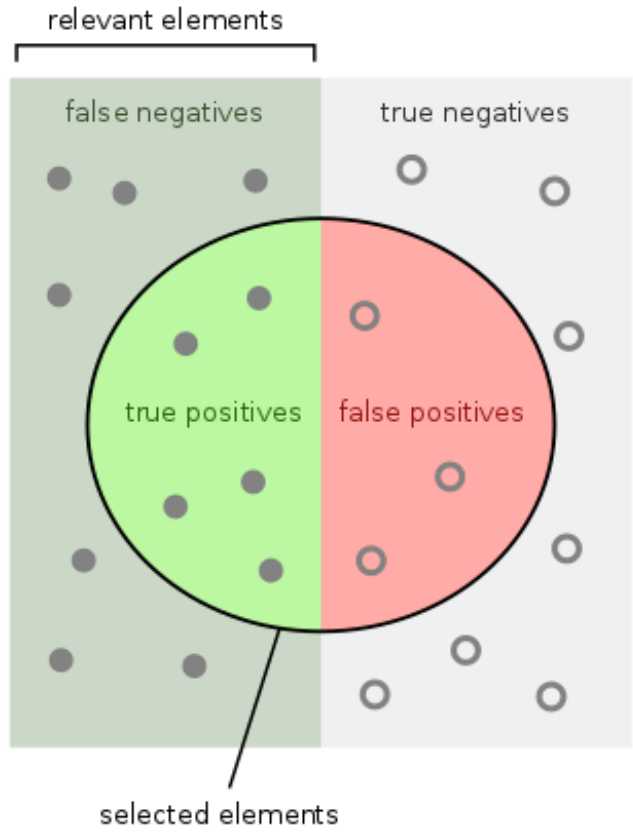
Measure model prediction **accuracy** on the testing set

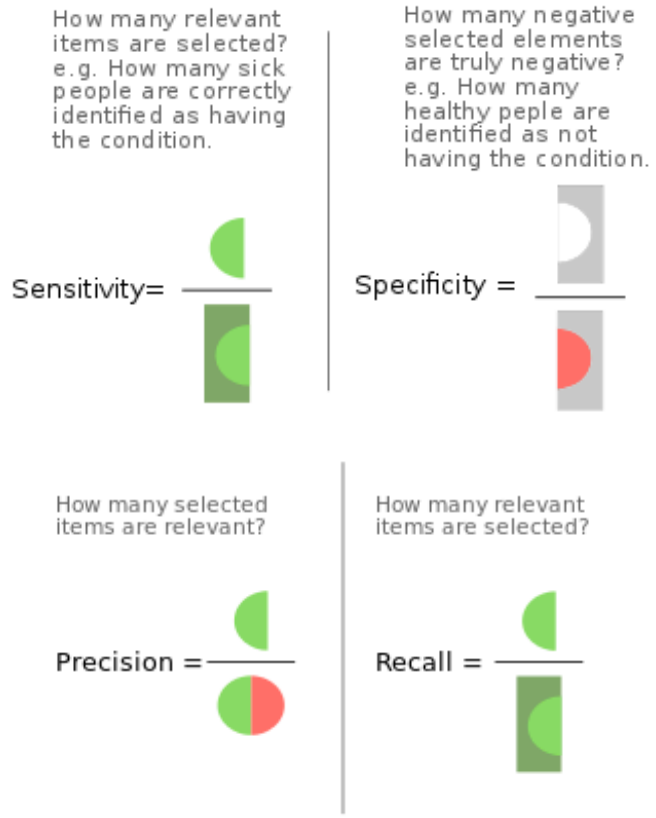
Classification Accuracy:

Precision

Sensitivity (Recall)

Specificity





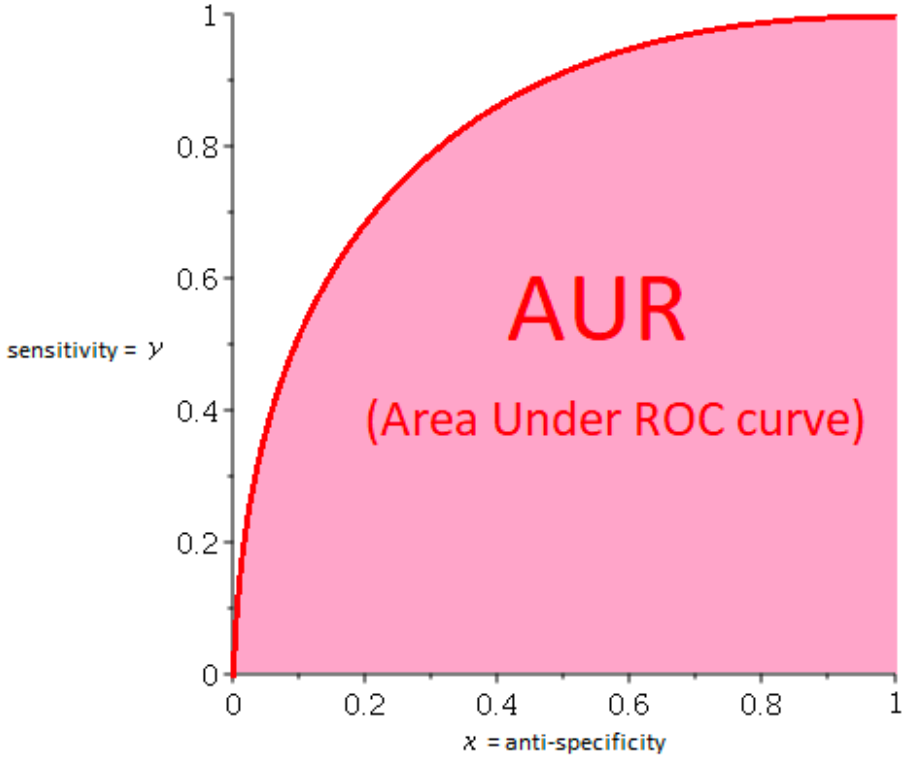
https://en.wikipedia.org/wiki/Sensitivity_and_specificity https://en.wikipedia.org/wiki/Precision_and_recall

Model Training and Testing

Receiver Operating Characteristic

As you increase your false positive rate, how quickly do you increase your true positive rate?

Goal is Area Under Curve = 1



https://towardsdatascience.com/understanding-auc-roc-curve-68b2303cc9c5
http://www.semspirit.com/artificial-intelligence/machine-learning/classification/classifier-evaluation/receiver-operating-characteristic-roc-curves/

Model Training and Testing

Measure model prediction **accuracy** on the testing set

Regression Accuracy (brief)

(Normalized) Root mean squared error

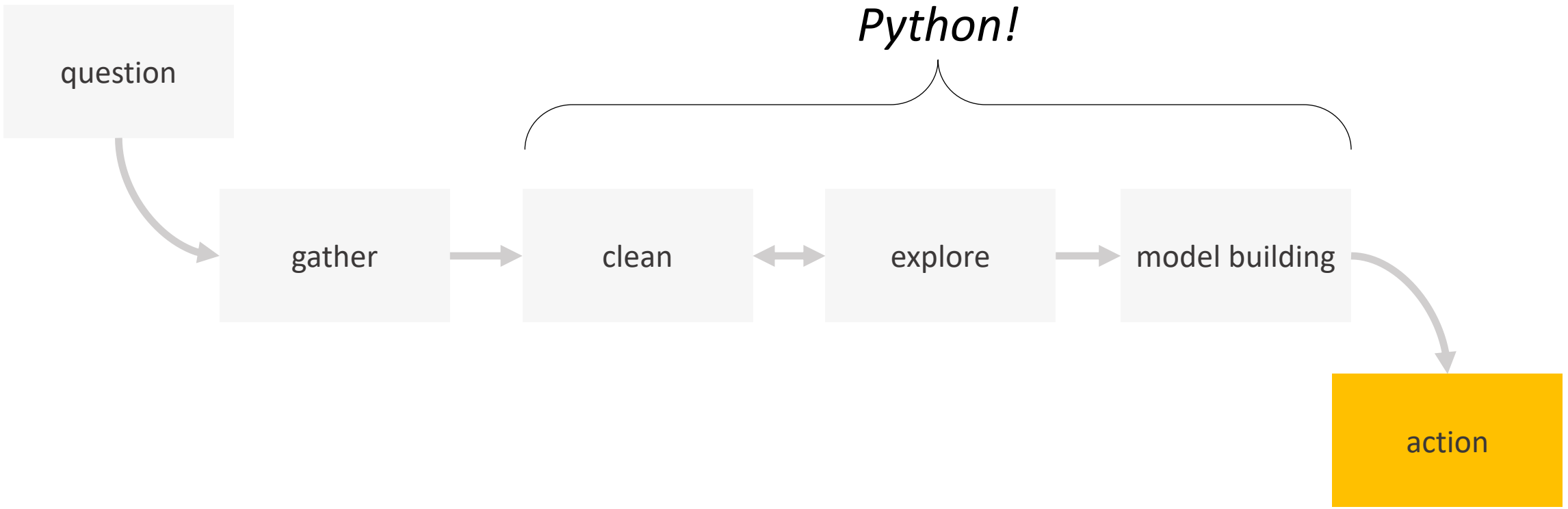
R^2

Model Training and Testing

Other train/test strategies

- K-fold cross-validation
- Leave-one-out validation

Data science workflow



Actionability of Data

Plant classifier could be used to help gardeners, scientists, or anyone with an interest in irises.

Did we fairly and equitably represent all *Iris* species?

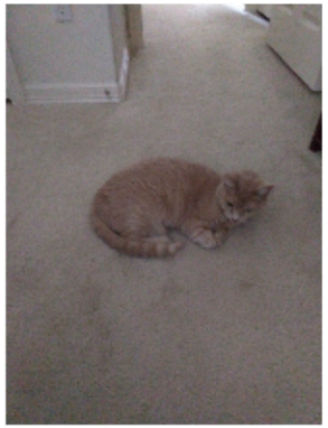
Does our model introduce bias into classification? If so, what consequences might there be?

Our *Iris* example is a bit contrived, but remember that **machine learning and data science drive actions daily** in a number of domains: healthcare, commerce, education, etc.

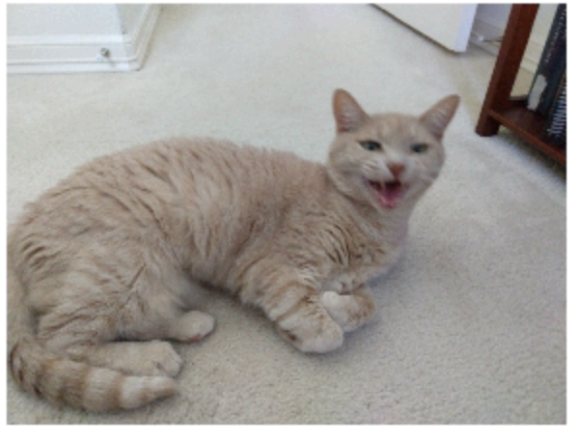
Classification Error

Classification Error

```
Probability% is <label>
 0.3375208 % is towel
 0.0611235 % is Aid
 0.0420474 % is Pekingese, Peke
 0.0291371 % is Angora rabbit
 0.0224534 % is tissue, toilet paper, bathroom tissue
 0.0200325 % is dough
 0.0150566 % is handbasin, washbowl, lavabo, wash-hand basin
 0.0145770 % is powder
 0.0145677 % is welcome mat
 0.0142751 % is nematode worm, roundworm
```



```
Probability% is <label>
 0.5441126 % is cat
 0.1973237 % is tabby cat
 0.1003607 % is cat
 0.0492031 % is cat, Siamese
 0.0410424 % is Highland white terrier
 0.0118241 % is heater
 0.0117978 % is catamount
 0.0083975 % is cairn terrier
 0.0074549 % is Pekingese, Peke
 0.0067524 % is cat
```



Classification Error

Hands on Exercises

https://github.com/kellyp2738/python_data_science

Clone or download > Download ZIP

Go to downloads folder and double click the ZIP file

Open Anaconda Navigator > click Jupyter Notebook

In the Jupyter notebook and select ‘Folder’ from the ‘New’ dropdown menu

Click the checkmark next to the Untitled Folder and select Rename from the menu bar. Name it “DataSci”.

Open DataSci, select Upload

Select all files from the Data Science folder in Downloads