

# Principles and Techniques of Data Science

**Data 100**

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## **Table of contents**

# Welcome

## About the Course Notes

This text offers supplementary resources to accompany lectures presented in the Spring 2025 Edition of the UC Berkeley course Data 100: Principles and Techniques of Data Science.

New notes will be added each week to accompany live lectures. See the full calendar of lectures on the [course website](#).

If you spot any typos or would like to suggest any changes, please email us at [data100.instructors@berkeley.edu](mailto:data100.instructors@berkeley.edu).

# 1 Introduction

## Learning Outcomes

- Acquaint yourself with the overarching goals of Data 100
- Understand the stages of the data science lifecycle

Data science is an interdisciplinary field with a variety of applications and offers great potential to address challenging societal issues. By building data science skills, you can empower yourself to participate in and drive conversations that shape your life and society as a whole, whether that be fighting against climate change, launching diversity initiatives, or more.

The field of data science is rapidly evolving; many of the key technical underpinnings in modern-day data science have been popularized during the early 21<sup>st</sup> century, and you will learn them throughout the course. It has a wide range of applications from science and medicine to sports.

While data science has immense potential to address challenging problems facing society by enhancing our critical thinking, it can also be used to obscure complex decisions and reinforce historical trends and biases. This course will implore you to consider the ethics of data science within its applications.

Data science is fundamentally human-centered and facilitates decision-making by quantitatively balancing tradeoffs. To quantify things reliably, we must use and analyze data appropriately, apply critical thinking and skepticism at every step of the way, and consider how our decisions affect others.

Ultimately, data science is the application of data-centric, computational, and inferential thinking to:

- Understand the world (science).
- Solve problems (engineering).

A true mastery of data science requires a deep theoretical understanding and strong grasp of domain expertise. This course will help you build on the former – specifically, the foundation of your technical knowledge, allowing you to take data and produce useful insights on the world’s most challenging and ambiguous problems.

### **i** Course Goals

- Prepare you for advanced Berkeley courses in **data management, machine learning, and statistics**.
- Enable you to launch a career as a data scientist by providing experience working with **real-world data, tools, and techniques**.
- Empower you to apply computational and inferential thinking to address **real-world problems**.

### **i** Some Topics We'll Cover

- pandas and NumPy
- Exploratory Data Analysis
- Regular Expressions
- Visualization
- Sampling
- Model Design and Loss Formulation
- Linear Regression
- Gradient Descent
- Logistic Regression
- Clustering
- PCA

### **i** Prerequisites

To ensure that you can get the most out of the course content, please make sure that you are familiar with:

- Using Python.
- Using Jupyter notebooks.
- Inference from Data 8.
- Linear algebra

To set you up for success, we've organized concepts in Data 100 around the **data science lifecycle**: an *iterative* process that encompasses the various statistical and computational building blocks of data science.

## 1.1 Data Science Lifecycle

The data science lifecycle is a *high-level overview* of the data science workflow. It's a cycle of stages that a data scientist should explore as they conduct a thorough analysis of a data-driven

problem.

There are many variations of the key ideas present in the data science lifecycle. In Data 100, we visualize the stages of the lifecycle using a flow diagram. Notice how there are two entry points.

### 1.1.1 Ask a Question

Whether by curiosity or necessity, data scientists constantly ask questions. For example, in the business world, data scientists may be interested in predicting the profit generated by a certain investment. In the field of medicine, they may ask whether some patients are more likely than others to benefit from a treatment.

Posing questions is one of the primary ways the data science lifecycle begins. It helps to fully define the question. Here are some things you should ask yourself before framing a question.

- What do we want to know?
  - A question that is too ambiguous may lead to confusion.
- What problems are we trying to solve?
  - The goal of asking a question should be clear in order to justify your efforts to stakeholders.
- What are the hypotheses we want to test?
  - This gives a clear perspective from which to analyze final results.
- What are the metrics for our success?
  - This establishes a clear point to know when to conclude the project.

### 1.1.2 Obtain Data

The second entry point to the lifecycle is by obtaining data. A careful analysis of any problem requires the use of data. Data may be readily available to us, or we may have to embark on a process to collect it. When doing so, it is crucial to ask the following:

- What data do we have, and what data do we need?
  - Define the units of the data (people, cities, points in time, etc.) and what features to measure.
- How will we sample more data?
  - Scrape the web, collect manually, run experiments, etc.

- Is our data representative of the population we want to study?
  - If our data is not representative of our population of interest, then we can come to incorrect conclusions.

Key procedures: *data acquisition, data cleaning*

### 1.1.3 Understand the Data

Raw data itself is not inherently useful. It's impossible to discern all the patterns and relationships between variables without carefully investigating them. Therefore, translating pure data into actionable insights is a key job of a data scientist. For example, we may choose to ask:

- How is our data organized, and what does it contain?
  - Knowing what the data says about the world helps us better understand the world.
- Do we have relevant data?
  - If the data we have collected is not useful to the question at hand, then we must collect more data.
- What are the biases, anomalies, or other issues with the data?
  - These can lead to many false conclusions if ignored, so data scientists must always be aware of these issues.
- How do we transform the data to enable effective analysis?
  - Data is not always easy to interpret at first glance, so a data scientist should strive to reveal the hidden insights.

Key procedures: *exploratory data analysis, data visualization.*

### 1.1.4 Understand the World

After observing the patterns in our data, we can begin answering our questions. This may require that we predict a quantity (machine learning) or measure the effect of some treatment (inference).

From here, we may choose to report our results, or possibly conduct more analysis. We may not be satisfied with our findings, or our initial exploration may have brought up new questions that require new data.

- What does the data say about the world?

- Given our models, the data will lead us to certain conclusions about the real world.
- Does it answer our questions or accurately solve the problem?
  - If our model and data can not accomplish our goals, then we must reform our question, model, or both.
- How robust are our conclusions and can we trust the predictions?
  - Inaccurate models can lead to false conclusions.

Key procedures: *model creation, prediction, inference*.

## 1.2 Conclusion

The data science lifecycle is meant to be a set of general guidelines rather than a hard set of requirements. In our journey exploring the lifecycle, we'll cover both the underlying theory and technologies used in data science. By the end of the course, we hope that you start to see yourself as a data scientist.

With that, we'll begin by introducing one of the most important tools in exploratory data analysis: **pandas**.



## 2 Pandas I

### Learning Outcomes

- Build familiarity with `pandas` and `pandas` syntax.
- Learn key data structures: `DataFrame`, `Series`, and `Index`.
- Understand methods for extracting data: `.loc`, `.iloc`, and `[]`.

In this sequence of lectures, we will dive right into things by having you explore and manipulate real-world data. We'll first introduce `pandas`, a popular Python library for interacting with **tabular data**.

### 2.1 Tabular Data

Data scientists work with data stored in a variety of formats. This class focuses primarily on *tabular data* — data that is stored in a table.

Tabular data is one of the most common systems that data scientists use to organize data. This is in large part due to the simplicity and flexibility of tables. Tables allow us to represent each **observation**, or instance of collecting data from an individual, as its own *row*. We can record each observation's distinct characteristics, or **features**, in separate *columns*.

To see this in action, we'll explore the `elections` dataset, which stores information about political candidates who ran for president of the United States in previous years.

In the `elections` dataset, each row (blue box) represents one instance of a candidate running for president in a particular year. For example, the first row represents Andrew Jackson running for president in the year 1824. Each column (yellow box) represents one characteristic piece of information about each presidential candidate. For example, the column named "Result" stores whether or not the candidate won the election.

Your work in Data 8 helped you grow very familiar with using and interpreting data stored in a tabular format. Back then, you used the `Table` class of the `datascience` library, a special programming library created specifically for Data 8 students.

In Data 100, we will be working with the programming library `pandas`, which is generally accepted in the data science community as the industry- and academia-standard tool for manipulating tabular data (as well as the inspiration for Petey, our panda bear mascot).

Using `pandas`, we can

- Arrange data in a tabular format.
- Extract useful information filtered by specific conditions.
- Operate on data to gain new insights.
- Apply NumPy functions to our data (our friends from Data 8).
- Perform vectorized computations to speed up our analysis (Lab 1).

## 2.2 Series, DataFrames, and Indices

To begin our work in `pandas`, we must first import the library into our Python environment. This will allow us to use `pandas` data structures and methods in our code.

```
# `pd` is the conventional alias for Pandas, as `np` is for NumPy
import pandas as pd
```

There are three fundamental data structures in `pandas`:

1. **Series**: 1D labeled array data; best thought of as columnar data.
2. **DataFrame**: 2D tabular data with rows and columns.
3. **Index**: A sequence of row/column labels.

`DataFrames`, `Series`, and `Indices` can be represented visually in the following diagram, which considers the first few rows of the `elections` dataset.

Notice how the **DataFrame** is a two-dimensional object — it contains both rows and columns. The **Series** above is a singular column of this **DataFrame**, namely the **Result** column. Both contain an **Index**, or a shared list of row labels (the integers from 0 to 4, inclusive).

### 2.2.1 Series

A **Series** represents a column of a **DataFrame**; more generally, it can be any 1-dimensional array-like object. It contains both:

- A sequence of **values** of the same type.
- A sequence of data labels called the **index**.

In the cell below, we create a **Series** named `s`.

```
s = pd.Series(["welcome", "to", "data 100"])
s
```

```
0    welcome
1         to
2    data 100
dtype: object
```

```
# Accessing data values within the Series
s.values
```

```
array(['welcome', 'to', 'data 100'], dtype=object)
```

```
# Accessing the Index of the Series
s.index
```

```
RangeIndex(start=0, stop=3, step=1)
```

By default, the `index` of a `Series` is a sequential list of integers beginning from 0. Optionally, a manually specified list of desired indices can be passed to the `index` argument.

```
s = pd.Series([-1, 10, 2], index = ["a", "b", "c"])
s
```

```
a    -1
b    10
c     2
dtype: int64
```

```
s.index
```

```
Index(['a', 'b', 'c'], dtype='object')
```

Indices can also be changed after initialization.

```
s.index = ["first", "second", "third"]
s
```

```
first    -1
second   10
third     2
dtype: int64
```

```
s.index
```

```
Index(['first', 'second', 'third'], dtype='object')
```

### 2.2.1.1 Selection in Series

Much like when working with NumPy arrays, we can select a single value or a set of values from a Series. To do so, there are three primary methods:

1. A single label.
2. A list of labels.
3. A filtering condition.

To demonstrate this, let's define a new Series `s`.

```
s = pd.Series([4, -2, 0, 6], index = ["a", "b", "c", "d"])
s
```

```
a    4
b   -2
c    0
d    6
dtype: int64
```

#### 2.2.1.1.1 A Single Label

```
# We return the value stored at the index label "a"
s["a"]
```

```
np.int64(4)
```

#### 2.2.1.1.2 A List of Labels

```
# We return a Series of the values stored at the index labels "a" and "c"
s[["a", "c"]]
```

```
a    4
c    0
dtype: int64
```

### 2.2.1.1.3 A Filtering Condition

Perhaps the most interesting (and useful) method of selecting data from a **Series** is by using a filtering condition.

First, we apply a boolean operation to the **Series**. This creates a **new Series of boolean values**.

```
# Filter condition: select all elements greater than 0
s > 0
```

```
a      True
b     False
c     False
d      True
dtype: bool
```

We then use this boolean condition to index into our original **Series**. **pandas** will select only the entries in the original **Series** that satisfy the condition.

```
s[s > 0]
```

```
a      4
d      6
dtype: int64
```

## 2.2.2 DataFrames

Typically, we will work with **Series** using the perspective that they are columns in a **DataFrame**. We can think of a **DataFrame** as a collection of **Series** that all share the same **Index**.

In Data 8, you encountered the **Table** class of the **datascience** library, which represented tabular data. In Data 100, we'll be using the **DataFrame** class of the **pandas** library.

### 2.2.2.1 Creating a DataFrame

There are many ways to create a **DataFrame**. Here, we will cover the most popular approaches:

1. From a CSV file.
2. Using a list and column name(s).

3. From a dictionary.
4. From a **Series**.

More generally, the syntax for creating a **DataFrame** is:

```
pandas.DataFrame(data, index, columns)
```

### 2.2.2.1.1 From a CSV file

In Data 100, our data are typically stored in a CSV (comma-separated values) file format. We can import a CSV file into a **DataFrame** by passing the data path as an argument to the following **pandas** function. `pd.read_csv("filename.csv")`

With our new understanding of **pandas** in hand, let's return to the **elections** dataset from before. Now, we can recognize that it is represented as a **pandas DataFrame**.

```
elections = pd.read_csv("data/elections.csv")
elections
```

		Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican		151271	loss	57.210122
1	1824	John Quincy Adams	Democratic-Republican		113142	win	42.789878
2	1828	Andrew Jackson	Democratic		642806	win	56.203927
3	1828	John Quincy Adams	National Republican		500897	loss	43.796073
4	1832	Andrew Jackson	Democratic		702735	win	54.574789
...	...	...	...		...	...	...
182	2024	Donald Trump	Republican		77303568	win	49.808629
183	2024	Kamala Harris	Democratic		75019230	loss	48.336772
184	2024	Jill Stein	Green		861155	loss	0.554864
185	2024	Robert Kennedy	Independent		756383	loss	0.487357
186	2024	Chase Oliver	Libertarian Party		650130	loss	0.418895

This code stores our **DataFrame** object in the **elections** variable. Upon inspection, our **elections DataFrame** has 182 rows and 6 columns (**Year**, **Candidate**, **Party**, **Popular Vote**, **Result**, **%**). Each row represents a single record — in our example, a presidential candidate from some particular year. Each column represents a single attribute or feature of the record.

### 2.2.2.1.2 Using a List and Column Name(s)

We'll now explore creating a `DataFrame` with data of our own.

Consider the following examples. The first code cell creates a `DataFrame` with a single column `Numbers`.

```
df_list = pd.DataFrame([1, 2, 3], columns=["Numbers"])
df_list
```

	Numbers
0	1
1	2
2	3

The second creates a `DataFrame` with the columns `Numbers` and `Description`. Notice how a 2D list of values is required to initialize the second `DataFrame` — each nested list represents a single row of data.

```
df_list = pd.DataFrame([1, "one"], [2, "two"], columns = ["Number", "Description"])
df_list
```

	Number	Description
0	1	one
1	2	two

### 2.2.2.1.3 From a Dictionary

A third (and more common) way to create a `DataFrame` is with a dictionary. The dictionary keys represent the column names, and the dictionary values represent the column values.

Below are two ways of implementing this approach. The first is based on specifying the columns of the `DataFrame`, whereas the second is based on specifying the rows of the `DataFrame`.

```
df_dict = pd.DataFrame({
    "Fruit": ["Strawberry", "Orange"],
    "Price": [5.49, 3.99]
})
df_dict
```

	Fruit	Price
0	Strawberry	5.49
1	Orange	3.99

```
df_dict = pd.DataFrame(
    [
        {"Fruit": "Strawberry", "Price": 5.49},
        {"Fruit": "Orange", "Price": 3.99}
    ]
)
df_dict
```

	Fruit	Price
0	Strawberry	5.49
1	Orange	3.99

#### 2.2.2.1.4 From a Series

Earlier, we explained how a **Series** was synonymous to a column in a **DataFrame**. It follows, then, that a **DataFrame** is equivalent to a collection of **Series**, which all share the same **Index**.

In fact, we can initialize a **DataFrame** by merging two or more **Series**. Consider the **Series** **s\_a** and **s\_b**.

```
# Notice how our indices, or row labels, are the same

s_a = pd.Series(["a1", "a2", "a3"], index = ["r1", "r2", "r3"])
s_b = pd.Series(["b1", "b2", "b3"], index = ["r1", "r2", "r3"])
```

We can turn individual **Series** into a **DataFrame** using two common methods (shown below):

```
pd.DataFrame(s_a)
```

0	
r1	a1
r2	a2
r3	a3



```
s_b.to_frame()
```

	0
r1	b1
r2	b2
r3	b3

To merge the two **Series** and specify their column names, we use the following syntax:

```
pd.DataFrame({
    "A-column": s_a,
    "B-column": s_b
})
```

	A-column	B-column
r1	a1	b1
r2	a2	b2
r3	a3	b3

### 2.2.3 Indices

On a more technical note, an index doesn't have to be an integer, nor does it have to be unique. For example, we can set the index of the **elections DataFrame** to be the name of presidential candidates.

```
# Creating a DataFrame from a CSV file and specifying the index column
elections = pd.read_csv("data/elections.csv", index_col = "Candidate")
elections
```

	Year	Party	Popular vote	Result	%
Candidate					
Andrew Jackson	1824	Democratic-Republican	151271	loss	57.210122
John Quincy Adams	1824	Democratic-Republican	113142	win	42.789878
Andrew Jackson	1828	Democratic	642806	win	56.203927
John Quincy Adams	1828	National Republican	500897	loss	43.796073
Andrew Jackson	1832	Democratic	702735	win	54.574789

	Year	Party	Popular vote	Result	%
Candidate					
...	...	...	...	...	...
Donald Trump	2024	Republican	77303568	win	49.808629
Kamala Harris	2024	Democratic	75019230	loss	48.336772
Jill Stein	2024	Green	861155	loss	0.554864
Robert Kennedy	2024	Independent	756383	loss	0.487357
Chase Oliver	2024	Libertarian Party	650130	loss	0.418895

We can also select a new column and set it as the index of the `DataFrame`. For example, we can set the index of the `elections DataFrame` to represent the candidate's party.

```
elections.reset_index(inplace = True) # Resetting the index so we can set it again
# This sets the index to the "Party" column
elections.set_index("Party")
```

	Candidate	Year	Popular vote	Result	%
Party					
Democratic-Republican	Andrew Jackson	1824	151271	loss	57.210122
Democratic-Republican	John Quincy Adams	1824	113142	win	42.789878
Democratic	Andrew Jackson	1828	642806	win	56.203927
National Republican	John Quincy Adams	1828	500897	loss	43.796073
Democratic	Andrew Jackson	1832	702735	win	54.574789
...	...	...	...	...	...
Republican	Donald Trump	2024	77303568	win	49.808629
Democratic	Kamala Harris	2024	75019230	loss	48.336772
Green	Jill Stein	2024	861155	loss	0.554864
Independent	Robert Kennedy	2024	756383	loss	0.487357
Libertarian Party	Chase Oliver	2024	650130	loss	0.418895

And, if we'd like, we can revert the index back to the default list of integers.

```
# This resets the index to be the default list of integer
elections.reset_index(inplace=True)
elections.index
```

```
RangeIndex(start=0, stop=187, step=1)
```

It is also important to note that the row labels that constitute an index don't have to be unique. While index values can be unique and numeric, acting as a row number, they can also be named and non-unique.

Here we see unique and numeric index values.

However, here the index values are not unique.

## 2.3 DataFrame Attributes: Index, Columns, and Shape

On the other hand, column names in a `DataFrame` are almost always unique. Looking back to the `elections` dataset, it wouldn't make sense to have two columns named `"Candidate"`. Sometimes, you'll want to extract these different values, in particular, the list of row and column labels.

For index/row labels, use `DataFrame.index`:

```
elections.set_index("Party", inplace = True)
elections.index
```

```
Index(['Democratic-Republican', 'Democratic-Republican', 'Democratic',
      'National Republican', 'Democratic', 'National Republican',
      'Anti-Masonic', 'Whig', 'Democratic', 'Whig',
      ...,
      'Green', 'Democratic', 'Republican', 'Libertarian', 'Green',
      'Republican', 'Democratic', 'Green', 'Independent',
      'Libertarian Party'],
      dtype='object', name='Party', length=187)
```

For column labels, use `DataFrame.columns`:

```
elections.columns
```

```
Index(['index', 'Candidate', 'Year', 'Popular vote', 'Result', '%'], dtype='object')
```

And for the shape of the `DataFrame`, we can use `DataFrame.shape` to get the number of rows followed by the number of columns:

```
elections.shape
```

```
(187, 6)
```

## 2.4 Slicing in DataFrames

Now that we've learned more about `DataFrame`s, let's dive deeper into their capabilities.

The API (Application Programming Interface) for the `DataFrame` class is enormous. In this section, we'll discuss several methods of the `DataFrame` API that allow us to extract subsets of data.

The simplest way to manipulate a `DataFrame` is to extract a subset of rows and columns, known as **slicing**.

Common ways we may want to extract data are grabbing:

- The first or last `n` rows in the `DataFrame`.
- Data with a certain label.
- Data at a certain position.

We will do so with four primary methods of the `DataFrame` class:

1. `.head` and `.tail`
2. `.loc`
3. `.iloc`
4. `[]`

### 2.4.1 Extracting data with `.head` and `.tail`

The simplest scenario in which we want to extract data is when we simply want to select the first or last few rows of the `DataFrame`.

To extract the first `n` rows of a `DataFrame` `df`, we use the syntax `df.head(n)`.

```
elections = pd.read_csv("data/elections.csv")
```

```
# Extract the first 5 rows of the DataFrame
elections.head(5)
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.210122
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.789878
2	1828	Andrew Jackson	Democratic	642806	win	56.203927
3	1828	John Quincy Adams	National Republican	500897	loss	43.796073
4	1832	Andrew Jackson	Democratic	702735	win	54.574789

Similarly, calling `df.tail(n)` allows us to extract the last `n` rows of the `DataFrame`.

```
# Extract the last 5 rows of the DataFrame
elections.tail(5)
```

	Year	Candidate	Party	Popular vote	Result	%
182	2024	Donald Trump	Republican	77303568	win	49.808629
183	2024	Kamala Harris	Democratic	75019230	loss	48.336772
184	2024	Jill Stein	Green	861155	loss	0.554864
185	2024	Robert Kennedy	Independent	756383	loss	0.487357
186	2024	Chase Oliver	Libertarian Party	650130	loss	0.418895

### 2.4.2 Label-based Extraction: Indexing with `.loc`

For the more complex task of extracting data with specific column or index labels, we can use `.loc`. The `.loc` accessor allows us to specify the **labels** of rows and columns we wish to extract. The **labels** (commonly referred to as the **indices**) are the bold text on the far *left* of a `DataFrame`, while the **column labels** are the column names found at the *top* of a `DataFrame`.

To grab data with `.loc`, we must specify the row and column label(s) where the data exists. The row labels are the first argument to the `.loc` function; the column labels are the second.

Arguments to `.loc` can be:

- A single value.
- A slice.
- A list.

For example, to select a single value, we can select the row labeled 0 and the column labeled `Candidate` from the `elections` `DataFrame`.

```
elections.loc[0, 'Candidate']
```

```
'Andrew Jackson'
```

Keep in mind that passing in just one argument as a single value will produce a `Series`. Below, we've extracted a subset of the "Popular vote" column as a `Series`.

```
elections.loc[[87, 25, 179], "Popular vote"]
```

```
87      15761254
25       848019
179     74216154
Name: Popular vote, dtype: int64
```

Note that if we pass "Popular vote" as a list, the output will be a `DataFrame`.

```
elections.loc[[87, 25, 179], ["Popular vote"]]
```

	Popular vote
87	15761254
25	848019
179	74216154

To select *multiple* rows and columns, we can use Python slice notation. Here, we select the rows from labels 0 to 3 and the columns from labels "Year" to "Popular vote". Notice that unlike Python slicing, `.loc` is *inclusive* of the right upper bound.

```
elections.loc[0:3, 'Year':'Popular vote']
```

	Year	Candidate	Party	Popular vote
0	1824	Andrew Jackson	Democratic-Republican	151271
1	1824	John Quincy Adams	Democratic-Republican	113142
2	1828	Andrew Jackson	Democratic	642806
3	1828	John Quincy Adams	National Republican	500897

Suppose that instead, we want to extract *all* column values for the first four rows in the `elections` `DataFrame`. The shorthand `:` is useful for this.

```
elections.loc[0:3, :]
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.210122

		Year	Candidate	Party	Popular vote	Result	%
1	1824	John Quincy Adams	Democratic-Republican		113142	win	42.789878
2	1828	Andrew Jackson	Democratic		642806	win	56.203927
3	1828	John Quincy Adams	National Republican		500897	loss	43.796073

We can use the same shorthand to extract all rows.

```
elections.loc[:, ["Year", "Candidate", "Result"]]
```

	Year	Candidate	Result
0	1824	Andrew Jackson	loss
1	1824	John Quincy Adams	win
2	1828	Andrew Jackson	win
3	1828	John Quincy Adams	loss
4	1832	Andrew Jackson	win
...	...	...	...
182	2024	Donald Trump	win
183	2024	Kamala Harris	loss
184	2024	Jill Stein	loss
185	2024	Robert Kennedy	loss
186	2024	Chase Oliver	loss

There are a couple of things we should note. Firstly, unlike conventional Python, **pandas** allows us to slice string values (in our example, the column labels). Secondly, slicing with `.loc` is *inclusive*. Notice how our resulting **DataFrame** includes every row and column between and including the slice labels we specified.

Equivalently, we can use a list to obtain multiple rows and columns in our **elections DataFrame**.

```
elections.loc[[0, 1, 2, 3], ['Year', 'Candidate', 'Party', 'Popular vote']]
```

		Year	Candidate	Party	Popular vote
0	1824	Andrew Jackson		Democratic-Republican	151271
1	1824	John Quincy Adams		Democratic-Republican	113142
2	1828	Andrew Jackson		Democratic	642806
3	1828	John Quincy Adams		National Republican	500897

Lastly, we can interchange list and slicing notation.

```
elections.loc[[0, 1, 2, 3], :]
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.210122
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.789878
2	1828	Andrew Jackson	Democratic	642806	win	56.203927
3	1828	John Quincy Adams	National Republican	500897	loss	43.796073

### 2.4.3 Integer-based Extraction: Indexing with `.iloc`

Slicing with `.iloc` works similarly to `.loc`. However, `.iloc` uses the *index positions* of rows and columns rather than the labels (think to yourself: `loc` uses **l**ables; `iloc` uses **i**ndices). The arguments to the `.iloc` function also behave similarly — single values, lists, indices, and any combination of these are permitted.

Let's begin reproducing our results from above. We'll begin by selecting the first presidential candidate in our `elections` `DataFrame`:

```
# elections.loc[0, "Candidate"] - Previous approach
elections.iloc[0, 1]
```

```
'Andrew Jackson'
```

Notice how the first argument to both `.loc` and `.iloc` are the same. This is because the row with a label of 0 is conveniently in the 0<sup>th</sup> (equivalently, the first position) of the `elections` `DataFrame`. Generally, this is true of any `DataFrame` where the row labels are incremented in ascending order from 0.

And, as before, if we were to pass in only one single value argument, our result would be a `Series`.

```
elections.iloc[[1,2,3],1]
```

```
1    John Quincy Adams
2      Andrew Jackson
3    John Quincy Adams
Name: Candidate, dtype: object
```

However, when we select the first four rows and columns using `.iloc`, we notice something.



```
# elections.loc[0:3, 'Year':'Popular vote'] - Previous approach
elections.iloc[0:4, 0:4]
```

		Year	Candidate	Party	Popular vote
0	1824	Andrew Jackson		Democratic-Republican	151271
1	1824	John Quincy Adams		Democratic-Republican	113142
2	1828	Andrew Jackson		Democratic	642806
3	1828	John Quincy Adams		National Republican	500897

Slicing is no longer inclusive in `.iloc` — it's *exclusive*. In other words, the right end of a slice is not included when using `.iloc`. This is one of the subtleties of `pandas` syntax; you will get used to it with practice.

List behavior works just as expected.

```
#elections.loc[[0, 1, 2, 3], ['Year', 'Candidate', 'Party', 'Popular vote']] - Previous Approach
elections.iloc[[0, 1, 2, 3], [0, 1, 2, 3]]
```

		Year	Candidate	Party	Popular vote
0	1824	Andrew Jackson		Democratic-Republican	151271
1	1824	John Quincy Adams		Democratic-Republican	113142
2	1828	Andrew Jackson		Democratic	642806
3	1828	John Quincy Adams		National Republican	500897

And just like with `.loc`, we can use a colon with `.iloc` to extract all rows or columns.

```
elections.iloc[:, 0:3]
```

		Year	Candidate	Party
0	1824	Andrew Jackson		Democratic-Republican
1	1824	John Quincy Adams		Democratic-Republican
2	1828	Andrew Jackson		Democratic
3	1828	John Quincy Adams		National Republican
4	1832	Andrew Jackson		Democratic
...	...	...		...
182	2024	Donald Trump		Republican
183	2024	Kamala Harris		Democratic

		Year	Candidate	Party
184	2024	Jill Stein		Green
185	2024	Robert Kennedy		Independent
186	2024	Chase Oliver		Libertarian Party

This discussion begs the question: when should we use `.loc` vs. `.iloc`? In most cases, `.loc` is generally safer to use. You can imagine `.iloc` may return incorrect values when applied to a dataset where the ordering of data can change. However, `.iloc` can still be useful — for example, if you are looking at a `DataFrame` of sorted movie earnings and want to get the median earnings for a given year, you can use `.iloc` to index into the middle.

Overall, it is important to remember that:

- `.loc` performs label-based extraction.
- `.iloc` performs integer-based extraction.

## 2.4.4 Context-dependent Extraction: Indexing with `[]`

The `[]` selection operator is the most baffling of all, yet the most commonly used. It only takes a single argument, which may be one of the following:

1. A slice of row numbers.
2. A list of column labels.
3. A single-column label.

That is, `[]` is *context-dependent*. Let's see some examples.

### 2.4.4.1 A slice of row numbers

Say we wanted the first four rows of our `elections DataFrame`.

```
elections[0:4]
```

		Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson		Democratic-Republican	151271	loss	57.210122
1	1824	John Quincy Adams		Democratic-Republican	113142	win	42.789878
2	1828	Andrew Jackson		Democratic	642806	win	56.203927
3	1828	John Quincy Adams		National Republican	500897	loss	43.796073

#### 2.4.4.2 A list of column labels

Suppose we now want the first four columns.

```
elections[["Year", "Candidate", "Party", "Popular vote"]]
```

		Year	Candidate	Party	Popular vote
0	1824	Andrew Jackson		Democratic-Republican	151271
1	1824	John Quincy Adams		Democratic-Republican	113142
2	1828	Andrew Jackson		Democratic	642806
3	1828	John Quincy Adams		National Republican	500897
4	1832	Andrew Jackson		Democratic	702735
...	...	...		...	...
182	2024	Donald Trump		Republican	77303568
183	2024	Kamala Harris		Democratic	75019230
184	2024	Jill Stein		Green	861155
185	2024	Robert Kennedy		Independent	756383
186	2024	Chase Oliver		Libertarian Party	650130

#### 2.4.4.3 A single-column label

Lastly, `[]` allows us to extract only the "Candidate" column.

```
elections["Candidate"]
```

```
0      Andrew Jackson
1    John Quincy Adams
2      Andrew Jackson
3    John Quincy Adams
4      Andrew Jackson
...
182     Donald Trump
183     Kamala Harris
184       Jill Stein
185    Robert Kennedy
186     Chase Oliver
Name: Candidate, Length: 187, dtype: object
```

The output is a **Series**! In this course, we'll become very comfortable with `[]`, especially for selecting columns. In practice, `[]` is much more common than `.loc`, especially since it is far more concise.

## 2.5 Parting Note

The **pandas** library is enormous and contains many useful functions. Here is a link to its [documentation](#). We certainly don't expect you to memorize each and every method of the library, and we will give you a reference sheet for exams.

The introductory Data 100 **pandas** lectures will provide a high-level view of the key data structures and methods that will form the foundation of your **pandas** knowledge. A goal of this course is to help you build your familiarity with the real-world programming practice of ... Googling! Answers to your questions can be found in documentation, Stack Overflow, etc. Being able to search for, read, and implement documentation is an important life skill for any data scientist.

With that, we will move on to Pandas II!

## 3 Pandas II

### Learning Outcomes

- Continue building familiarity with **pandas** syntax.
- Extract data from a **DataFrame** using conditional selection.
- Recognize situations where aggregation is useful and identify the correct technique for performing an aggregation.

Last time, we introduced the **pandas** library as a toolkit for processing data. We learned the **DataFrame** and **Series** data structures, familiarized ourselves with the basic syntax for manipulating tabular data, and began writing our first lines of **pandas** code.

In this lecture, we'll start to dive into some advanced **pandas** syntax. You may find it helpful to follow along with a notebook of your own as we walk through these new pieces of code.

We'll start by loading the **babynames** dataset.

```
# This code pulls census data and loads it into a DataFrame
# We won't cover it explicitly in this class, but you are welcome to explore it on your own
import pandas as pd
import numpy as np
import urllib.request
import os.path
import zipfile

data_url = "https://www.ssa.gov/oact/babynames/state/namesbystate.zip"
local_filename = "data/babynamesbystate.zip"
if not os.path.exists(local_filename): # If the data exists don't download again
    with urllib.request.urlopen(data_url) as resp, open(local_filename, 'wb') as f:
        f.write(resp.read())

zf = zipfile.ZipFile(local_filename, 'r')

ca_name = 'STATE.CA.TXT'
field_names = ['State', 'Sex', 'Year', 'Name', 'Count']
with zf.open(ca_name) as fh:
    babynames = pd.read_csv(fh, header=None, names=field_names)
```

```
babynames.head()
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

### 3.1 Conditional Selection

Conditional selection allows us to select a subset of rows in a `DataFrame` that satisfy some specified condition.

To understand how to use conditional selection, we must look at another possible input of the `.loc` and `[]` methods – a boolean array, which is simply an array or `Series` where each element is either `True` or `False`. This boolean array must have a length equal to the number of rows in the `DataFrame`. It will return all rows that correspond to a value of `True` in the array. We used a very similar technique when performing conditional extraction from a `Series` in the last lecture.

To see this in action, let's select all even-indexed rows in the first 10 rows of our `DataFrame`.

```
# Ask yourself: why is :9 is the correct slice to select the first 10 rows?
babynames_first_10_rows = babynames.loc[:9, :]

# Notice how we have exactly 10 elements in our boolean array argument
babynames_first_10_rows[[True, False, True, False, True, False, True, False, True, False]]
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
2	CA	F	1910	Dorothy	220
4	CA	F	1910	Frances	134
6	CA	F	1910	Evelyn	126
8	CA	F	1910	Virginia	101

We can perform a similar operation using `.loc`.

```
babynames_first_10_rows.loc[[True, False, True, False, True, False, True, False, True, False]]
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
2	CA	F	1910	Dorothy	220
4	CA	F	1910	Frances	134
6	CA	F	1910	Evelyn	126
8	CA	F	1910	Virginia	101

These techniques worked well in this example, but you can imagine how tedious it might be to list out `True` and `False` for every row in a larger `DataFrame`. To make things easier, we can instead provide a logical condition as an input to `.loc` or `[]` that returns a boolean array with the necessary length.

For example, to return all names associated with F sex:

```
# First, use a logical condition to generate a boolean array
logical_operator = (babynames["Sex"] == "F")

# Then, use this boolean array to filter the DataFrame
babynames[logical_operator].head()
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

Recall from the previous lecture that `.head()` will return only the first few rows in the `DataFrame`. In reality, `babynames[logical_operator]` contains as many rows as there are entries in the original `babynames` `DataFrame` with sex "F".

Here, `logical_operator` evaluates to a `Series` of boolean values with length 407428.

```
print("There are a total of {} values in 'logical_operator'".format(len(logical_operator)))
```

```
There are a total of 407428 values in 'logical_operator'
```

Rows starting at row 0 and ending at row 239536 evaluate to **True** and are thus returned in the **DataFrame**. Rows from 239537 onwards evaluate to **False** and are omitted from the output.

```
print("The 0th item in this 'logical_operator' is: {}".format(logical_operator.iloc[0]))
print("The 239536th item in this 'logical_operator' is: {}".format(logical_operator.iloc[239536]))
print("The 239537th item in this 'logical_operator' is: {}".format(logical_operator.iloc[239537]))
```

```
The 0th item in this 'logical_operator' is: True
The 239536th item in this 'logical_operator' is: True
The 239537th item in this 'logical_operator' is: False
```

Passing a **Series** as an argument to **babynames[]** has the same effect as using a boolean array. In fact, the **[]** selection operator can take a boolean **Series**, array, and list as arguments. These three are used interchangeably throughout the course.

We can also use **.loc** to achieve similar results.

```
babynames.loc[babynames["Sex"] == "F"].head()
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

Boolean conditions can be combined using various bitwise operators, allowing us to filter results by multiple conditions. In the table below, **p** and **q** are boolean arrays or **Series**.

	Symbol	Usage	Meaning
~	~p		Returns negation of p
	p   q		p OR q
&	p & q		p AND q
^	p ^ q		p XOR q (exclusive or)

When combining multiple conditions with logical operators, we surround each individual condition with a set of parenthesis **()**. This imposes an order of operations on **pandas** evaluating your logic and can avoid code erroring.

For example, if we want to return data on all names with sex "F" born before the year 2000, we can write:



```
babynames[(babynames["Sex"] == "F") & (babynames["Year"] < 2000)].head()
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

Note that we're working with **Series**, so using **and** in place of **&**, or **or** in place of **|** will error.

```
# This line of code will raise a ValueError
# babynames[(babynames["Sex"] == "F") and (babynames["Year"] < 2000)].head()
```

If we want to return data on all names with sex "F" *or* all born before the year 2000, we can write:

```
babynames[(babynames["Sex"] == "F") | (babynames["Year"] < 2000)].head()
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

Boolean array selection is a useful tool, but can lead to overly verbose code for complex conditions. In the example below, our boolean condition is long enough to extend for several lines of code.

```
# Note: The parentheses surrounding the code make it possible to break the code on to multiple lines
(
    babynames[(babynames["Name"] == "Bella") |
               (babynames["Name"] == "Alex") |
               (babynames["Name"] == "Ani") |
               (babynames["Name"] == "Lisa")]
).head()
```

	State	Sex	Year	Name	Count
6289	CA	F	1923	Bella	5
7512	CA	F	1925	Bella	8
12368	CA	F	1932	Lisa	5
14741	CA	F	1936	Lisa	8
17084	CA	F	1939	Lisa	5

Fortunately, **pandas** provides many alternative methods for constructing boolean filters.

The `.isin` function is one such example. This method evaluates if the values in a **Series** are contained in a different sequence (list, array, or **Series**) of values. In the cell below, we achieve equivalent results to the **DataFrame** above with far more concise code.

```
names = ["Bella", "Alex", "Narges", "Lisa"]
babynames["Name"].isin(names).head()
```

```
0    False
1    False
2    False
3    False
4    False
Name: Name, dtype: bool
```

```
babynames[babynames["Name"].isin(names)].head()
```

	State	Sex	Year	Name	Count
6289	CA	F	1923	Bella	5
7512	CA	F	1925	Bella	8
12368	CA	F	1932	Lisa	5
14741	CA	F	1936	Lisa	8
17084	CA	F	1939	Lisa	5

The function `str.startswith` can be used to define a filter based on string values in a **Series** object. It checks to see if string values in a **Series** start with a particular character.

```
# Identify whether names begin with the letter "N"
babynames["Name"].str.startswith("N").head()
```

```

0    False
1    False
2    False
3    False
4    False
Name: Name, dtype: bool

```

```

# Extracting names that begin with the letter "N"
babynames[babynames["Name"].str.startswith("N")].head()

```

	State	Sex	Year	Name	Count
76	CA	F	1910	Norma	23
83	CA	F	1910	Nellie	20
127	CA	F	1910	Nina	11
198	CA	F	1910	Nora	6
310	CA	F	1911	Nellie	23

## 3.2 Adding, Removing, and Modifying Columns

In many data science tasks, we may need to change the columns contained in our `DataFrame` in some way. Fortunately, the syntax to do so is fairly straightforward.

To add a new column to a `DataFrame`, we use a syntax similar to that used when accessing an existing column. Specify the name of the new column by writing `df["column"]`, then assign this to a `Series` or array containing the values that will populate this column.

```

# Create a Series of the length of each name.
babynames["name_lengths"] = babynames["Name"].str.len()

# Add a column named "name_lengths" that includes the length of each name
babynames["name_lengths"] = babynames["name_lengths"]
babynames.head(5)

```

	State	Sex	Year	Name	Count	name_lengths
0	CA	F	1910	Mary	295	4
1	CA	F	1910	Helen	239	5
2	CA	F	1910	Dorothy	220	7
3	CA	F	1910	Margaret	163	8

	State	Sex	Year	Name	Count	name_lengths
4	CA	F	1910	Frances	134	7

If we need to later modify an existing column, we can do so by referencing this column again with the syntax `df["column"]`, then re-assigning it to a new **Series** or array of the appropriate length.

```
# Modify the "name_lengths" column to be one less than its original value
babynames["name_lengths"] = babynames["name_lengths"] - 1
babynames.head()
```

	State	Sex	Year	Name	Count	name_lengths
0	CA	F	1910	Mary	295	3
1	CA	F	1910	Helen	239	4
2	CA	F	1910	Dorothy	220	6
3	CA	F	1910	Margaret	163	7
4	CA	F	1910	Frances	134	6

We can rename a column using the `.rename()` method. It takes in a dictionary that maps old column names to their new ones.

```
# Rename "name_lengths" to "Length"
babynames = babynames.rename(columns={"name_lengths": "Length"})
babynames.head()
```

	State	Sex	Year	Name	Count	Length
0	CA	F	1910	Mary	295	3
1	CA	F	1910	Helen	239	4
2	CA	F	1910	Dorothy	220	6
3	CA	F	1910	Margaret	163	7
4	CA	F	1910	Frances	134	6

If we want to remove a column or row of a **DataFrame**, we can call the `.drop` ([documentation](#)) method. Use the **axis** parameter to specify whether a column or row should be dropped. Unless otherwise specified, **pandas** will assume that we are dropping a row by default.

```
# Drop our new "Length" column from the DataFrame
babynames = babynames.drop("Length", axis="columns")
babynames.head(5)
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

Notice that we *re-assigned* `babynames` to the result of `babynames.drop(...)`. This is a subtle but important point: **pandas** table operations **do not occur in-place**. Calling `df.drop(...)` will output a *copy* of `df` with the row/column of interest removed without modifying the original `df` table.

In other words, if we simply call:

```
# This creates a copy of `babynames` and removes the column "Name"...
babynames.drop("Name", axis="columns")

# ...but the original `babynames` is unchanged!
# Notice that the "Name" column is still present
babynames.head(5)
```

	State	Sex	Year	Name	Count
0	CA	F	1910	Mary	295
1	CA	F	1910	Helen	239
2	CA	F	1910	Dorothy	220
3	CA	F	1910	Margaret	163
4	CA	F	1910	Frances	134

### 3.3 Useful Utility Functions

**pandas** contains an extensive library of functions that can help shorten the process of setting and getting information from its data structures. In the following section, we will give overviews of each of the main utility functions that will help us in Data 100.

Discussing all functionality offered by `pandas` could take an entire semester! We will walk you through the most commonly-used functions and encourage you to explore and experiment on your own.

- NumPy and built-in function support
- `.shape`
- `.size`
- `.describe()`
- `.sample()`
- `.value_counts()`
- `.unique()`
- `.sort_values()`

The `pandas` [documentation](#) will be a valuable resource in Data 100 and beyond.

### 3.3.1 NumPy

`pandas` is designed to work well with NumPy, the framework for array computations you encountered in [Data 8](#). Just about any NumPy function can be applied to `pandas` `DataFrames` and `Series`.

```
# Pull out the number of babies named Yash each year
yash_count = babynames[babynames["Name"] == "Yash"]["Count"]
yash_count.head()
```

```
331824      8
334114      9
336390     11
338773     12
341387     10
Name: Count, dtype: int64
```

```
# Average number of babies named Yash each year
np.mean(yash_count)
```

```
np.float64(17.142857142857142)
```

```
# Max number of babies named Yash born in any one year
np.max(yash_count)
```

```
np.int64(29)
```

### 3.3.2 .shape and .size

`.shape` and `.size` are attributes of `Series` and `DataFrames` that measure the “amount” of data stored in the structure. Calling `.shape` returns a tuple containing the number of rows and columns present in the `DataFrame` or `Series`. `.size` is used to find the total number of elements in a structure, equivalent to the number of rows times the number of columns.

Many functions strictly require the dimensions of the arguments along certain axes to match. Calling these dimension-finding functions is much faster than counting all of the items by hand.

```
# Return the shape of the DataFrame, in the format (num_rows, num_columns)
babynames.shape
```

```
(407428, 5)
```

```
# Return the size of the DataFrame, equal to num_rows * num_columns
babynames.size
```

```
2037140
```

### 3.3.3 .describe()

If many statistics are required from a `DataFrame` (minimum value, maximum value, mean value, etc.), then `.describe()` ([documentation](#)) can be used to compute all of them at once.

```
babynames.describe()
```

	Year	Count
count	407428.000000	407428.000000
mean	1985.733609	79.543456
std	27.007660	293.698654
min	1910.000000	5.000000
25%	1969.000000	7.000000
50%	1992.000000	13.000000
75%	2008.000000	38.000000
max	2022.000000	8260.000000

A different set of statistics will be reported if `.describe()` is called on a `Series`.

```
babynames["Sex"].describe()
```

```
count      407428
unique         2
top          F
freq      239537
Name: Sex, dtype: object
```

### 3.3.4 .sample()

As we will see later in the semester, random processes are at the heart of many data science techniques (for example, train-test splits, bootstrapping, and cross-validation). `.sample()` ([documentation](#)) lets us quickly select random entries (a row if called from a `DataFrame`, or a value if called from a `Series`).

By default, `.sample()` selects entries *without* replacement. Pass in the argument `replace=True` to sample with replacement.

```
# Sample a single row
babynames.sample()
```

	State	Sex	Year	Name	Count
73262	CA	F	1975	Marty	6

Naturally, this can be chained with other methods and operators (`iloc`, etc.).

```
# Sample 5 random rows, and select all columns after column 2
babynames.sample(5).iloc[:, 2:]
```

	Year	Name	Count
204233	2013	Jarely	8
210541	2015	Aliya	36
187159	2009	Brea	13
272410	1961	Gregory	1835
124341	1993	Sophie	78



```
# Randomly sample 4 names from the year 2000, with replacement, and select all columns after
babynames[babynames["Year"] == 2000].sample(4, replace = True).iloc[:, 2:]
```

	Year	Name	Count
150479	2000	Allissa	17
152044	2000	Hania	6
151591	2000	Nitya	8
151543	2000	Kaycie	8

### 3.3.5 .value\_counts()

The `Series.value_counts()` ([documentation](#)) method counts the number of occurrence of each unique value in a `Series`. In other words, it *counts* the number of times each unique *value* appears. This is often useful for determining the most or least common entries in a `Series`.

In the example below, we can determine the name with the most years in which at least one person has taken that name by counting the number of times each name appears in the "Name" column of `babynames`. Note that the return value is also a `Series`.

```
babynames["Name"].value_counts().head()
```

```
Name
Jean      223
Francis   221
Guadalupe 218
Jessie     217
Marion     214
Name: count, dtype: int64
```

### 3.3.6 .unique()

If we have a `Series` with many repeated values, then `.unique()` ([documentation](#)) can be used to identify only the *unique* values. Here we return an array of all the names in `babynames`.

```
babynames["Name"].unique()
```

```
array(['Mary', 'Helen', 'Dorothy', ..., 'Zae', 'Zai', 'Zayvier'],
      shape=(20437,), dtype=object)
```

### 3.3.7 .sort\_values()

Ordering a `DataFrame` can be useful for isolating extreme values. For example, the first 5 entries of a row sorted in descending order (that is, from highest to lowest) are the largest 5 values. `.sort_values` ([documentation](#)) allows us to order a `DataFrame` or `Series` by a specified column. We can choose to either receive the rows in **ascending** order (default) or **descending** order.

```
# Sort the "Count" column from highest to lowest
babynames.sort_values(by="Count", ascending=False).head()
```

	State	Sex	Year	Name	Count
268041	CA	M	1957	Michael	8260
267017	CA	M	1956	Michael	8258
317387	CA	M	1990	Michael	8246
281850	CA	M	1969	Michael	8245
283146	CA	M	1970	Michael	8196

Unlike when calling `.value_counts()` on a `DataFrame`, we do not need to explicitly specify the column used for sorting when calling `.value_counts()` on a `Series`. We can still specify the ordering paradigm – that is, whether values are sorted in ascending or descending order.

```
# Sort the "Name" Series alphabetically
babynames["Name"].sort_values(ascending=True).head()
```

```
366001      Aadan
384005      Aadan
369120      Aadan
398211  Aadarsh
370306      Aaden
Name: Name, dtype: object
```

## 3.4 Parting Note

Manipulating `DataFrames` is not a skill that is mastered in just one day. Due to the flexibility of `pandas`, there are many different ways to get from point A to point B. We recommend trying multiple different ways to solve the same problem to gain even more practice and reach that point of mastery sooner.

Next, we will start digging deeper into the mechanics behind grouping data.

## 4 Pandas III

### Learning Outcomes

- Perform advanced aggregation using `.groupby()`
- Use the `pd.pivot_table` method to construct a pivot table
- Perform simple merges between DataFrames using `pd.merge()`

We will introduce the concept of aggregating data – we will familiarize ourselves with `GroupBy` objects and used them as tools to consolidate and summarize a `DataFrame`. In this lecture, we will explore working with the different aggregation functions and dive into some advanced `.groupby` methods to show just how powerful of a resource they can be for understanding our data. We will also introduce other techniques for data aggregation to provide flexibility in how we manipulate our tables.

### 4.1 Custom Sorts

First, let's finish our discussion about sorting. Let's try to solve a sorting problem using different approaches. Assume we want to find the longest baby names and sort our data accordingly.

We'll start by loading the `babynames` dataset. Note that this dataset is filtered to only contain data from California.

```
# This code pulls census data and loads it into a DataFrame
# We won't cover it explicitly in this class, but you are welcome to explore it on your own
import warnings
warnings.simplefilter(action='ignore', category=FutureWarning)

import pandas as pd
import numpy as np
import urllib.request
import os.path
import zipfile

data_url = "https://www.ssa.gov/oact/babynames/state/namesbystate.zip"
```

```

local_filename = "data/babynamesbystate.zip"
if not os.path.exists(local_filename): # If the data exists don't download again
    with urllib.request.urlopen(data_url) as resp, open(local_filename, 'wb') as f:
        f.write(resp.read())

zf = zipfile.ZipFile(local_filename, 'r')

ca_name = 'STATE.CA.TXT'
field_names = ['State', 'Sex', 'Year', 'Name', 'Count']
with zf.open(ca_name) as fh:
    babynames = pd.read_csv(fh, header=None, names=field_names)

babynames.tail(10)

```

	State	Sex	Year	Name	Count
407418	CA	M	2022	Zach	5
407419	CA	M	2022	Zadkiel	5
407420	CA	M	2022	Zae	5
407421	CA	M	2022	Zai	5
407422	CA	M	2022	Zay	5
407423	CA	M	2022	Zayvier	5
407424	CA	M	2022	Zia	5
407425	CA	M	2022	Zora	5
407426	CA	M	2022	Zuriel	5
407427	CA	M	2022	Zylo	5

#### 4.1.1 Approach 1: Create a Temporary Column

One method to do this is to first start by creating a column that contains the lengths of the names.

```

# Create a Series of the length of each name
babynames["name_lengths"] = babynames["Name"].str.len()

# Add a column named "name_lengths" that includes the length of each name
babynames["name_lengths"] = babynames["name_lengths"]
babynames.head(5)

```

	State	Sex	Year	Name	Count	name_lengths
0	CA	F	1910	Mary	295	4
1	CA	F	1910	Helen	239	5
2	CA	F	1910	Dorothy	220	7
3	CA	F	1910	Margaret	163	8
4	CA	F	1910	Frances	134	7

We can then sort the `DataFrame` by that column using `.sort_values()`:

```
# Sort by the temporary column
babynames = babynames.sort_values(by="name_lengths", ascending=False)
babynames.head(5)
```

	State	Sex	Year	Name	Count	name_lengths
316886	CA	M	1989	Franciscojavier	6	15
327472	CA	M	1993	Ryanchristopher	5	15
337477	CA	M	1997	Ryanchristopher	5	15
321792	CA	M	1991	Ryanchristopher	7	15
313977	CA	M	1988	Franciscojavier	10	15

Finally, we can drop the `name_length` column from `babynames` to prevent our table from getting cluttered.

```
# Drop the 'name_length' column
babynames = babynames.drop("name_lengths", axis='columns')
babynames.head(5)
```

	State	Sex	Year	Name	Count
316886	CA	M	1989	Franciscojavier	6
327472	CA	M	1993	Ryanchristopher	5
337477	CA	M	1997	Ryanchristopher	5
321792	CA	M	1991	Ryanchristopher	7
313977	CA	M	1988	Franciscojavier	10

#### 4.1.2 Approach 2: Sorting using the key Argument

Another way to approach this is to use the `key` argument of `.sort_values()`. Here we can specify that we want to sort "Name" values by their length.

```
babynames.sort_values("Name", key=lambda x: x.str.len(), ascending=False).head()
```

	State	Sex	Year	Name	Count
321792	CA	M	1991	Ryanchristopher	7
337477	CA	M	1997	Ryanchristopher	5
312543	CA	M	1987	Franciscojavier	5
102505	CA	F	1986	Mariadelosangel	5
327472	CA	M	1993	Ryanchristopher	5

### 4.1.3 Approach 3: Sorting using the map Function

We can also use the `map` function on a `Series` to solve this. Say we want to sort the `babynames` table by the number of "dr"s and "ea"s in each "Name". We'll define the function `dr_ea_count` to help us out.

```
# First, define a function to count the number of times "dr" or "ea" appear in each name
def dr_ea_count(string):
    return string.count('dr') + string.count('ea')

# Then, use `map` to apply `dr_ea_count` to each name in the "Name" column
babynames["dr_ea_count"] = babynames["Name"].map(dr_ea_count)

# Sort the DataFrame by the new "dr_ea_count" column so we can see our handiwork
babynames = babynames.sort_values(by="dr_ea_count", ascending=False)
babynames.head()
```

	State	Sex	Year	Name	Count	dr_ea_count
101976	CA	F	1986	Deandrea	6	3
115957	CA	F	1990	Deandrea	5	3
308131	CA	M	1985	Deandrea	6	3
131029	CA	F	1994	Leandrea	5	3
108731	CA	F	1988	Deandrea	5	3

We can drop the `dr_ea_count` once we're done using it to maintain a neat table.

```
# Drop the `dr_ea_count` column
babynames = babynames.drop("dr_ea_count", axis = 'columns')
babynames.head(5)
```

	State	Sex	Year	Name	Count
101976	CA	F	1986	Deandrea	6
115957	CA	F	1990	Deandrea	5
308131	CA	M	1985	Deandrea	6
131029	CA	F	1994	Leandrea	5
108731	CA	F	1988	Deandrea	5

## 4.2 Aggregating Data with `.groupby`

Up until this point, we have been working with individual rows of `DataFrames`. As data scientists, we often wish to investigate trends across a larger *subset* of our data. For example, we may want to compute some summary statistic (the mean, median, sum, etc.) for a group of rows in our `DataFrame`. To do this, we'll use `pandas` `GroupBy` objects. Our goal is to group together rows that fall under the same category and perform an operation that aggregates across all rows in the category.

Let's say we wanted to aggregate all rows in `babynames` for a given year.

```
babynames.groupby("Year")
```

```
<pandas.core.groupby.generic.DataFrameGroupBy object at 0x000001EFDD248050>
```

What does this strange output mean? Calling `.groupby` ([documentation](#)) has generated a `GroupBy` object. You can imagine this as a set of “mini” sub-`DataFrames`, where each subframe contains all of the rows from `babynames` that correspond to a particular year.

The diagram below shows a simplified view of `babynames` to help illustrate this idea.

We can't work with a `GroupBy` object directly – that is why you saw that strange output earlier rather than a standard view of a `DataFrame`. To actually manipulate values within these “mini” `DataFrames`, we'll need to call an *aggregation method*. This is a method that tells `pandas` how to aggregate the values within the `GroupBy` object. Once the aggregation is applied, `pandas` will return a normal (now grouped) `DataFrame`.

The first aggregation method we'll consider is `.agg`. The `.agg` method takes in a function as its argument; this function is then applied to each column of a “mini” grouped `DataFrame`. We end up with a new `DataFrame` with one aggregated row per subframe. Let's see this in action by finding the `sum` of all counts for each year in `babynames` – this is equivalent to finding the number of babies born in each year.

```
babynames[["Year", "Count"]].groupby("Year").agg("sum").head(5)
```

	Count
Year	
1910	9163
1911	9983
1912	17946
1913	22094
1914	26926

We can relate this back to the diagram we used above. Remember that the diagram uses a simplified version of `babynames`, which is why we see smaller values for the summed counts.

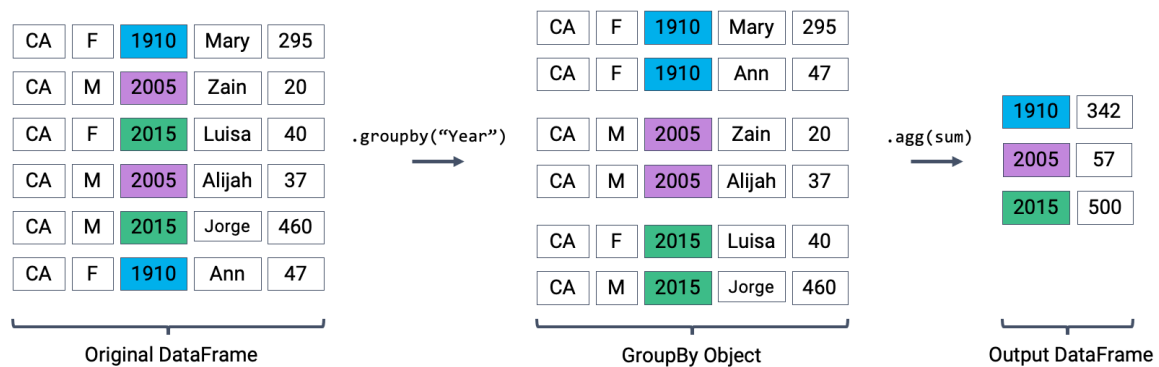


Figure 4.1: Performing an aggregation

Calling `.agg` has condensed each subframe back into a single row. This gives us our final output: a `DataFrame` that is now indexed by "Year", with a single row for each unique year in the original `babynames` `DataFrame`.

There are many different aggregation functions we can use, all of which are useful in different applications.

```
babynames[["Year", "Count"]].groupby("Year").agg("min").head(5)
```

	Count
Year	
1910	5



	Count
Year	
1911	5
1912	5
1913	5
1914	5

```
babynames[["Year", "Count"]].groupby("Year").agg("max").head(5)
```

	Count
Year	
1910	295
1911	390
1912	534
1913	614
1914	773

```
# Same result, but now we explicitly tell pandas to only consider the "Count" column when summing
babynames.groupby("Year")[["Count"]].agg("sum").head(5)
```

	Count
Year	
1910	9163
1911	9983
1912	17946
1913	22094
1914	26926

There are many different aggregations that can be applied to the grouped data. The primary requirement is that an aggregation function must:

- Take in a **Series** of data (a single column of the grouped subframe).
- Return a single value that aggregates this **Series**.

### 4.2.1 Aggregation Functions

Because of this fairly broad requirement, **pandas** offers many ways of computing an aggregation.

**In-built** Python operations – such as `sum`, `max`, and `min` – are automatically recognized by `pandas`.

```
# What is the minimum count for each name in any year?
babynames.groupby("Name")[["Count"]].agg("min").head()
```

	Count
Name	
Aadan	5
Aadarsh	6
Aaden	10
Aadhav	6
Aadhini	6

```
# What is the largest single-year count of each name?
babynames.groupby("Name")[["Count"]].agg("max").head()
```

	Count
Name	
Aadan	7
Aadarsh	6
Aaden	158
Aadhav	8
Aadhini	6

As mentioned previously, functions from the NumPy library, such as `np.mean`, `np.max`, `np.min`, and `np.sum`, are also fair game in `pandas`.

```
# What is the average count for each name across all years?
babynames.groupby("Name")[["Count"]].agg("mean").head()
```

	Count
Name	
Aadan	6.000000
Aadarsh	6.000000
Aaden	46.214286
Aadhav	6.750000

	Count
Name	
Aadhini	6.000000

`pandas` also offers a number of in-built functions. Functions that are native to `pandas` can be referenced using their string name within a call to `.agg`. Some examples include:

- `.agg("sum")`
- `.agg("max")`
- `.agg("min")`
- `.agg("mean")`
- `.agg("first")`
- `.agg("last")`

The latter two entries in this list – `"first"` and `"last"` – are unique to `pandas`. They return the first or last entry in a subframe column. Why might this be useful? Consider a case where *multiple* columns in a group share identical information. To represent this information in the grouped output, we can simply grab the first or last entry, which we know will be identical to all other entries.

Let's illustrate this with an example. Say we add a new column to `babynames` that contains the first letter of each name.

```
# Imagine we had an additional column, "First Letter". We'll explain this code next week
babynames["First Letter"] = babynames["Name"].str[0]

# We construct a simplified DataFrame containing just a subset of columns
babynames_new = babynames[["Name", "First Letter", "Year"]]
babynames_new.head()
```

	Name	First Letter	Year
101976	Deandrea	D	1986
115957	Deandrea	D	1990
308131	Deandrea	D	1985
131029	Leandrea	L	1994
108731	Deandrea	D	1988

If we form groups for each name in the dataset, `"First Letter"` will be the same for all members of the group. This means that if we simply select the first entry for `"First Letter"` in the group, we'll represent all data in that group.

We can use a dictionary to apply different aggregation functions to each column during grouping.

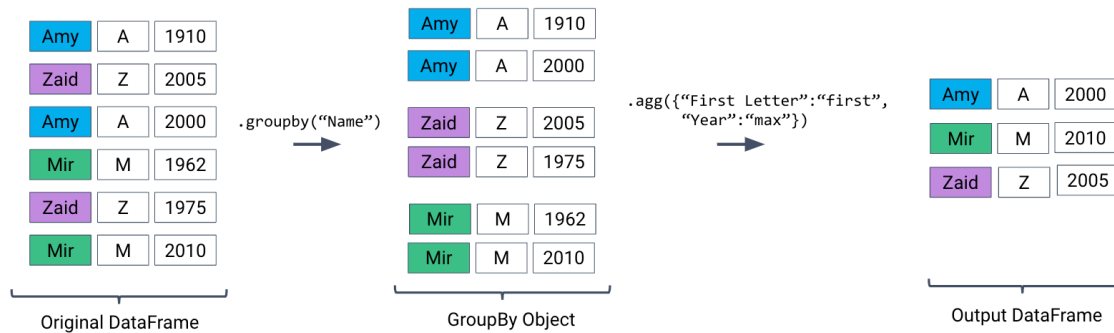


Figure 4.2: Aggregating using “first”

```
babynames_new.groupby("Name").agg({"First Letter":"first", "Year":"max"}).head()
```

	First Letter	Year
Name		
Aadan	A	2014
Aadarsh	A	2019
Aaden	A	2020
Aadhav	A	2019
Aadhini	A	2022

## 4.2.2 Plotting Birth Counts

Let's use `.agg` to find the total number of babies born in each year. Recall that using `.agg` with `.groupby()` follows the format: `df.groupby(column_name).agg(aggregation_function)`. The line of code below gives us the total number of babies born in each year.

```
babynames.groupby("Year")["Count"].agg(sum).head(5)
# Alternative 1
# babynames.groupby("Year")["Count"].sum()
# Alternative 2
# babynames.groupby("Year").sum(numeric_only=True)
```

	Count
Year	
1910	9163
1911	9983
1912	17946
1913	22094
1914	26926

Here's an illustration of the process:

Plotting the `DataFrame` we obtain tells an interesting story.

```
import plotly.express as px
puzzle2 = babynames.groupby("Year")[["Count"]].agg("sum")
px.line(puzzle2, y = "Count")
```

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**A word of warning:** we made an enormous assumption when we decided to use this dataset to estimate birth rate. According to [this article from the Legislative Analyst Office](#), the true number of babies born in California in 2020 was 421,275. However, our plot shows 362,882 babies — what happened?

### 4.2.3 Summary of the `.groupby()` Function

A `groupby` operation involves some combination of **splitting a `DataFrame` into grouped subframes**, **applying a function**, and **combining the results**.

For some arbitrary `DataFrame` `df` below, the code `df.groupby("year").agg(sum)` does the following:

- **Splits** the `DataFrame` into sub-`DataFrames` with rows belonging to the same year.
- **Applies** the `sum` function to each column of each sub-`DataFrame`.
- **Combines** the results of `sum` into a single `DataFrame`, indexed by `year`.

### 4.2.4 Revisiting the .agg() Function

.agg() can take in any function that aggregates several values into one summary value. Some commonly-used aggregation functions can even be called directly, without explicit use of .agg(). For example, we can call .mean() on .groupby():

```
babynames.groupby("Year").mean().head()
```

We can now put this all into practice. Say we want to find the baby name with sex “F” that has fallen in popularity the most in California. To calculate this, we can first create a metric: “Ratio to Peak” (RTP). The RTP is the ratio of babies born with a given name in 2022 to the *maximum* number of babies born with the name in *any* year.

Let’s start with calculating this for one baby, “Jennifer”.

```
# We filter by babies with sex "F" and sort by "Year"
f_babynames = babynames[babynames["Sex"] == "F"]
f_babynames = f_babynames.sort_values(["Year"])

# Determine how many Jennifers were born in CA per year
jenn_counts_series = f_babynames[f_babynames["Name"] == "Jennifer"]["Count"]

# Determine the max number of Jennifers born in a year and the number born in 2022
# to calculate RTP
max_jenn = max(f_babynames[f_babynames["Name"] == "Jennifer"]["Count"])
curr_jenn = f_babynames[f_babynames["Name"] == "Jennifer"]["Count"].iloc[-1]
rtp = curr_jenn / max_jenn
rtp
```

```
np.float64(0.018796372629843364)
```

By creating a function to calculate RTP and applying it to our DataFrame by using .groupby(), we can easily compute the RTP for all names at once!

```
def ratio_to_peak(series):
    return series.iloc[-1] / max(series)

#Using .groupby() to apply the function
rtp_table = f_babynames.groupby("Name")[["Year", "Count"]].agg(ratio_to_peak)
rtp_table.head()
```

	Year	Count
Name		
Aadhini	1.0	1.000000
Aadhira	1.0	0.500000
Aadhya	1.0	0.660000
Aadya	1.0	0.586207
Aahana	1.0	0.269231

In the rows shown above, we can see that every row shown has a **Year** value of 1.0.

This is the “**pandas**-ification” of logic you saw in Data 8. Much of the logic you’ve learned in Data 8 will serve you well in Data 100.

## 4.2.5 Nuisance Columns

Note that you must be careful with which columns you apply the `.agg()` function to. If we were to apply our function to the table as a whole by doing `f_babynames.groupby("Name").agg(ratio_to_peak)`, executing our `.agg()` call would result in a `TypeError`.

We can avoid this issue (and prevent unintentional loss of data) by explicitly selecting column(s) we want to apply our aggregation function to **BEFORE** calling `.agg()`,

## 4.2.6 Renaming Columns After Grouping

By default, `.groupby` will not rename any aggregated columns. As we can see in the table above, the aggregated column is still named `Count` even though it now represents the RTP. For better readability, we can rename `Count` to `Count RTP`

```
rtp_table = rtp_table.rename(columns = {"Count": "Count RTP"})
rtp_table
```

	Year	Count RTP
Name		
Aadhini	1.0	1.000000
Aadhira	1.0	0.500000
Aadhya	1.0	0.660000
Aadya	1.0	0.586207
Aahana	1.0	0.269231
...	...	...

Name	Year	Count RTP
Zyanya	1.0	0.466667
Zyla	1.0	1.000000
Zylah	1.0	1.000000
Zyra	1.0	1.000000
Zyrah	1.0	0.833333

### 4.2.7 Some Data Science Payoff

By sorting `rtp_table`, we can see the names whose popularity has decreased the most.

```
rtp_table = rtp_table.rename(columns = {"Count": "Count RTP"})
rtp_table.sort_values("Count RTP").head()
```

Name	Year	Count RTP
Debra	1.0	0.001260
Debbie	1.0	0.002815
Carol	1.0	0.003180
Tammy	1.0	0.003249
Susan	1.0	0.003305

To visualize the above `DataFrame`, let's look at the line plot below:

```
import plotly.express as px
px.line(f_babynames[f_babynames["Name"] == "Debra"], x = "Year", y = "Count")
```

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We can get the list of the top 10 names and then plot popularity with the following code:

```
top10 = rtp_table.sort_values("Count RTP").head(10).index
px.line(
    f_babynames[f_babynames["Name"].isin(top10)],
    x = "Year",
    y = "Count",
    color = "Name"
)
```



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As a quick exercise, consider what code would compute the total number of babies with each name.

```
babynames.groupby("Name")[["Count"]].agg("sum").head()
# alternative solution:
# babynames.groupby("Name")[["Count"]].sum()
```

		Count
Name		
Aadan		18
Aadarsh		6
Aaden		647
Aadhav		27
Aadhini		6

## 4.3 .groupby(), Continued

We'll work with the `elections` `DataFrame` again.

```
import pandas as pd
import numpy as np

elections = pd.read_csv("data/elections.csv")
elections.head(5)
```

		Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican		151271	loss	57.210122
1	1824	John Quincy Adams	Democratic-Republican		113142	win	42.789878
2	1828	Andrew Jackson	Democratic		642806	win	56.203927
3	1828	John Quincy Adams	National Republican		500897	loss	43.796073
4	1832	Andrew Jackson	Democratic		702735	win	54.574789

### 4.3.1 Raw GroupBy Objects

The result of `groupby` applied to a `DataFrame` is a `DataFrameGroupBy` object, **not** a `DataFrame`.

```
grouped_by_year = elections.groupby("Year")
type(grouped_by_year)
```

```
pandas.core.groupby.generic.DataFrameGroupBy
```

There are several ways to look into `DataFrameGroupBy` objects:

```
grouped_by_party = elections.groupby("Party")
grouped_by_party.groups
```

```
{'American': [22, 126], 'American Independent': [115, 119, 124], 'Anti-Masonic': [6], 'Anti-Slavery': [78], 'Free Soil': [15, 18], 'Green': [149, 155, 156, 165, 170, 177, 181, 184], 'Greenback': [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200]}
```

```
grouped_by_party.get_group("Socialist")
```

	Year	Candidate	Party	Popular vote	Result	%
58	1904	Eugene V. Debs	Socialist	402810	loss	2.985897
62	1908	Eugene V. Debs	Socialist	420852	loss	2.850866
66	1912	Eugene V. Debs	Socialist	901551	loss	6.004354
71	1916	Allan L. Benson	Socialist	590524	loss	3.194193
76	1920	Eugene V. Debs	Socialist	913693	loss	3.428282
85	1928	Norman Thomas	Socialist	267478	loss	0.728623
88	1932	Norman Thomas	Socialist	884885	loss	2.236211
92	1936	Norman Thomas	Socialist	187910	loss	0.412876
95	1940	Norman Thomas	Socialist	116599	loss	0.234237
102	1948	Norman Thomas	Socialist	139569	loss	0.286312

### 4.3.2 Other GroupBy Methods

There are many aggregation methods we can use with `.agg`. Some useful options are:

- `.mean`: creates a new `DataFrame` with the mean value of each group
- `.sum`: creates a new `DataFrame` with the sum of each group

- `.max` and `.min`: creates a new **DataFrame** with the maximum/minimum value of each group
- `.first` and `.last`: creates a new **DataFrame** with the first/last row in each group
- `.size`: creates a new **Series** with the number of entries in each group
- `.count`: creates a new **DataFrame** with the number of entries, excluding missing values.

Let's illustrate some examples by creating a **DataFrame** called `df`.

```
df = pd.DataFrame({'letter': ['A', 'A', 'B', 'C', 'C', 'C'],
                  'num': [1, 2, 3, 4, np.nan, 4],
                  'state': [np.nan, 'tx', 'fl', 'hi', np.nan, 'ak']})
df
```

	letter	num	state
0	A	1.0	NaN
1	A	2.0	tx
2	B	3.0	fl
3	C	4.0	hi
4	C	NaN	NaN
5	C	4.0	ak

Note the slight difference between `.size()` and `.count()`: while `.size()` returns a **Series** and counts the number of entries including the missing values, `.count()` returns a **DataFrame** and counts the number of entries in each column *excluding missing values*.

```
df.groupby("letter").size()
```

```
letter
A      2
B      1
C      3
dtype: int64
```

```
df.groupby("letter").count()
```

	num	state
letter		
A	2	1

	num	state
letter		
B	1	1
C	2	2

You might recall that the `value_counts()` function in the previous note does something similar. It turns out `value_counts()` and `groupby.size()` are the same, except `value_counts()` sorts the resulting Series in descending order automatically.

```
df["letter"].value_counts()
```

```
letter
C      3
A      2
B      1
Name: count, dtype: int64
```

These (and other) aggregation functions are so common that **pandas** allows for writing shorthand. Instead of explicitly stating the use of `.agg`, we can call the function directly on the `GroupBy` object.

For example, the following are equivalent:

- `elections.groupby("Candidate").agg(mean)`
- `elections.groupby("Candidate").mean()`

There are many other methods that **pandas** supports. You can check them out on the [pandas documentation](#).

### 4.3.3 Filtering by Group

Another common use for `GroupBy` objects is to filter data by group.

`groupby.filter` takes an argument `func`, where `func` is a function that:

- Takes a `DataFrame` object as input
- Returns a single `True` or `False`.

`groupby.filter` applies `func` to each group/sub-`DataFrame`:

- If `func` returns `True` for a group, then all rows belonging to the group are preserved.
- If `func` returns `False` for a group, then all rows belonging to that group are filtered out.

In other words, sub-DataFrames that correspond to `True` are returned in the final result, whereas those with a `False` value are not. Importantly, `groupby.filter` is different from `groupby.agg` in that an *entire* sub-DataFrame is returned in the final DataFrame, not just a single row. As a result, `groupby.filter` preserves the original indices and the column we grouped on does **NOT** become the index!

To illustrate how this happens, let's go back to the `elections` dataset. Say we want to identify “tight” election years – that is, we want to find all rows that correspond to election years where all candidates in that year won a similar portion of the total vote. Specifically, let's find all rows corresponding to a year where no candidate won more than 45% of the total vote.

In other words, we want to:

- Find the years where the maximum % in that year is less than 45%
- Return all DataFrame rows that correspond to these years

For each year, we need to find the maximum % among *all* rows for that year. If this maximum % is lower than 45%, we will tell `pandas` to keep all rows corresponding to that year.

```
elections.groupby("Year").filter(lambda sf: sf["%"].max() < 45).head(9)
```

	Year	Candidate	Party	Popular vote	Result	%
23	1860	Abraham Lincoln	Republican	1855993	win	39.699408
24	1860	John Bell	Constitutional Union	590901	loss	12.639283
25	1860	John C. Breckinridge	Southern Democratic	848019	loss	18.138998
26	1860	Stephen A. Douglas	Northern Democratic	1380202	loss	29.522311
66	1912	Eugene V. Debs	Socialist	901551	loss	6.004354
67	1912	Eugene W. Chafin	Prohibition	208156	loss	1.386325
68	1912	Theodore Roosevelt	Progressive	4122721	loss	27.457433
69	1912	William Taft	Republican	3486242	loss	23.218466
70	1912	Woodrow Wilson	Democratic	6296284	win	41.933422

What's going on here? In this example, we've defined our filtering function, `func`, to be `lambda sf: sf["%"].max() < 45`. This filtering function will find the maximum "%" value among all entries in the grouped sub-DataFrame, which we call `sf`. If the maximum value is less than 45, then the filter function will return `True` and all rows in that grouped sub-DataFrame will appear in the final output DataFrame.

Examine the DataFrame above. Notice how, in this preview of the first 9 rows, all entries from the years 1860 and 1912 appear. This means that in 1860 and 1912, no candidate in that year won more than 45% of the total vote.

You may ask: how is the `groupby.filter` procedure different to the boolean filtering we've seen previously? Boolean filtering considers *individual* rows when applying a boolean condition. For example, the code `elections[elections["%"] < 45]` will check the "%" value of every single row in `elections`; if it is less than 45, then that row will be kept in the output. `groupby.filter`, in contrast, applies a boolean condition *across* all rows in a group. If not all rows in that group satisfy the condition specified by the filter, the entire group will be discarded in the output.

#### 4.3.4 Aggregation with lambda Functions

What if we wish to aggregate our `DataFrame` using a non-standard function – for example, a function of our own design? We can do so by combining `.agg` with `lambda` expressions.

Let's first consider a puzzle to jog our memory. We will attempt to find the `Candidate` from each `Party` with the highest % of votes.

A naive approach may be to group by the `Party` column and aggregate by the maximum.

```
elections.groupby("Party").agg(max).head(10)
```

	Year	Candidate	Popular vote	Result	%
Party					
American	1976	Thomas J. Anderson	873053	loss	21.554001
American Independent	1976	Lester Maddox	9901118	loss	13.571218
Anti-Masonic	1832	William Wirt	100715	loss	7.821583
Anti-Monopoly	1884	Benjamin Butler	134294	loss	1.335838
Citizens	1980	Barry Commoner	233052	loss	0.270182
Communist	1932	William Z. Foster	103307	loss	0.261069
Constitution	2016	Michael Peroutka	203091	loss	0.152398
Constitutional Union	1860	John Bell	590901	loss	12.639283
Democratic	2024	Woodrow Wilson	81268924	win	61.344703
Democratic-Republican	1824	John Quincy Adams	151271	win	57.210122

This approach is clearly wrong – the `DataFrame` claims that Woodrow Wilson won the presidency in 2020.

Why is this happening? Here, the `max` aggregation function is taken over every column *independently*. Among Democrats, `max` is computing:

- The most recent `Year` a Democratic candidate ran for president (2020)
- The `Candidate` with the alphabetically “largest” name (“Woodrow Wilson”)
- The `Result` with the alphabetically “largest” outcome (“win”)

Instead, let's try a different approach. We will:

1. Sort the **DataFrame** so that rows are in descending order of %
2. Group by **Party** and select the first row of each sub-**DataFrame**

While it may seem unintuitive, sorting **elections** by descending order of % is extremely helpful. If we then group by **Party**, the first row of each **GroupBy** object will contain information about the **Candidate** with the highest voter %.

```
elections_sorted_by_percent = elections.sort_values("%", ascending=False)
elections_sorted_by_percent.head(5)
```

		Year	Candidate	Party	Popular vote	Result	%
114	1964	Lyndon Johnson	Democratic	43127041	win	61.344703	
91	1936	Franklin Roosevelt	Democratic	27752648	win	60.978107	
120	1972	Richard Nixon	Republican	47168710	win	60.907806	
79	1920	Warren Harding	Republican	16144093	win	60.574501	
133	1984	Ronald Reagan	Republican	54455472	win	59.023326	

```
elections_sorted_by_percent.groupby("Party").agg(lambda x : x.iloc[0]).head(10)

# Equivalent to the below code
# elections_sorted_by_percent.groupby("Party").agg('first').head(10)
```

		Year	Candidate	Popular vote	Result	%
Party						
American		1856	Millard Fillmore	873053	loss	21.554001
American Independent		1968	George Wallace	9901118	loss	13.571218
Anti-Masonic		1832	William Wirt	100715	loss	7.821583
Anti-Monopoly		1884	Benjamin Butler	134294	loss	1.335838
Citizens		1980	Barry Commoner	233052	loss	0.270182
Communist		1932	William Z. Foster	103307	loss	0.261069
Constitution		2008	Chuck Baldwin	199750	loss	0.152398
Constitutional Union		1860	John Bell	590901	loss	12.639283
Democratic		1964	Lyndon Johnson	43127041	win	61.344703
Democratic-Republican		1824	Andrew Jackson	151271	loss	57.210122

Here's an illustration of the process:

Notice how our code correctly determines that Lyndon Johnson from the Democratic Party has the highest voter %.

More generally, `lambda` functions are used to design custom aggregation functions that aren't pre-defined by Python. The input parameter `x` to the `lambda` function is a `GroupBy` object. Therefore, it should make sense why `lambda x : x.iloc[0]` selects the first row in each groupby object.

In fact, there's a few different ways to approach this problem. Each approach has different tradeoffs in terms of readability, performance, memory consumption, complexity, etc. We've given a few examples below.

**Note:** Understanding these alternative solutions is not required. They are given to demonstrate the vast number of problem-solving approaches in `pandas`.

```
# Using the idxmax function
best_per_party = elections.loc[elections.groupby('Party')['%'].idxmax()]
best_per_party.head(5)
```

		Year	Candidate	Party	Popular vote	Result	%
22	1856	Millard Fillmore	American		873053	loss	21.554001
115	1968	George Wallace	American Independent		9901118	loss	13.571218
6	1832	William Wirt	Anti-Masonic		100715	loss	7.821583
38	1884	Benjamin Butler	Anti-Monopoly		134294	loss	1.335838
127	1980	Barry Commoner	Citizens		233052	loss	0.270182

```
# Using the .drop_duplicates function
best_per_party2 = elections.sort_values('%').drop_duplicates(['Party'], keep='last')
best_per_party2.head(5)
```

		Year	Candidate	Party	Popular vote	Result	%
148	1996	John Hagelin	Natural Law		113670	loss	0.118219
164	2008	Chuck Baldwin	Constitution		199750	loss	0.152398
110	1956	T. Coleman Andrews	States' Rights		107929	loss	0.174883
147	1996	Howard Phillips	Taxpayers		184656	loss	0.192045
136	1988	Lenora Fulani	New Alliance		217221	loss	0.237804

## 4.4 Aggregating Data with Pivot Tables

We know now that `.groupby` gives us the ability to group and aggregate data across our `DataFrame`. The examples above formed groups using just one column in the `DataFrame`.



It's possible to group by multiple columns at once by passing in a list of column names to `.groupby`.

Let's consider the `babynames` dataset again. In this problem, we will find the total number of baby names associated with each sex for each year. To do this, we'll group by *both* the `"Year"` and `"Sex"` columns.

```
babynames.head()
```

	State	Sex	Year	Name	Count	First Letter
101976	CA	F	1986	Deandrea	6	D
115957	CA	F	1990	Deandrea	5	D
308131	CA	M	1985	Deandrea	6	D
131029	CA	F	1994	Leandrea	5	L
108731	CA	F	1988	Deandrea	5	D

```
# Find the total number of baby names associated with each sex for each
# year in the data
babynames.groupby(["Year", "Sex"])["Count"].agg(sum).head(6)
```

			Count
	Year	Sex	
1910		F	5950
		M	3213
1911		F	6602
		M	3381
1912		F	9804
		M	8142

Notice that both `"Year"` and `"Sex"` serve as the index of the `DataFrame` (they are both rendered in bold). We've created a *multi-index DataFrame* where two different index values, the year and sex, are used to uniquely identify each row.

This isn't the most intuitive way of representing this data – and, because multi-indexed `DataFrames` have multiple dimensions in their index, they can often be difficult to use.

Another strategy to aggregate across two columns is to create a pivot table. You saw these back in [Data 8](#). One set of values is used to create the index of the pivot table; another set is used to define the column names. The values contained in each cell of the table correspond to the aggregated data for each index-column pair.

Here's an illustration of the process:

The best way to understand pivot tables is to see one in action. Let's return to our original goal of summing the total number of names associated with each combination of year and sex. We'll call the pandas `.pivot_table` method to create a new table.

```
# The `pivot_table` method is used to generate a Pandas pivot table
import numpy as np
babynames.pivot_table(
    index = "Year",
    columns = "Sex",
    values = "Count",
    aggfunc = "sum",
).head(5)
```

Year	Sex	
	F	M
1910	5950	3213
1911	6602	3381
1912	9804	8142
1913	11860	10234
1914	13815	13111

Looks a lot better! Now, our **DataFrame** is structured with clear index-column combinations. Each entry in the pivot table represents the summed count of names for a given combination of "Year" and "Sex".

Let's take a closer look at the code implemented above.

- `index = "Year"` specifies the column name in the original **DataFrame** that should be used as the index of the pivot table
- `columns = "Sex"` specifies the column name in the original **DataFrame** that should be used to generate the columns of the pivot table
- `values = "Count"` indicates what values from the original **DataFrame** should be used to populate the entry for each index-column combination
- `aggfunc = np.sum` tells **pandas** what function to use when aggregating the data specified by `values`. Here, we are summing the name counts for each pair of "Year" and "Sex"

We can even include multiple values in the index or columns of our pivot tables.

```

babynames_pivot = babynames.pivot_table(
    index="Year",      # the rows (turned into index)
    columns="Sex",     # the column values
    values=["Count", "Name"],
    aggfunc="max",     # group operation
)
babynames_pivot.head(6)

```

	Count		Name		
	Sex	F	M	F	M
	Year				
1910	295	237	Yvonne	William	
1911	390	214	Zelma	Willis	
1912	534	501	Yvonne	Woodrow	
1913	584	614	Zelma	Yoshio	
1914	773	769	Zelma	Yoshio	
1915	998	1033	Zita	Yukio	

Note that each row provides the number of girls and number of boys having that year's most common name, and also lists the alphabetically largest girl name and boy name. The counts for number of girls/boys in the resulting `DataFrame` do not correspond to the names listed. For example, in 1910, the most popular girl name is given to 295 girls, but that name was likely not Yvonne.

## 4.5 Joining Tables

When working on data science projects, we're unlikely to have absolutely all the data we want contained in a single `DataFrame` – a real-world data scientist needs to grapple with data coming from multiple sources. If we have access to multiple datasets with related information, we can join two or more tables into a single `DataFrame`.

To put this into practice, we'll revisit the `elections` dataset.

```
elections.head(5)
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.210122
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.789878

	Year	Candidate	Party	Popular vote	Result	%
2	1828	Andrew Jackson	Democratic	642806	win	56.203927
3	1828	John Quincy Adams	National Republican	500897	loss	43.796073
4	1832	Andrew Jackson	Democratic	702735	win	54.574789

Say we want to understand the popularity of the names of each presidential candidate in 2022. To do this, we'll need the combined data of **babynames** and **elections**.

We'll start by creating a new column containing the first name of each presidential candidate. This will help us join each name in **elections** to the corresponding name data in **babynames**.

```
# This `str` operation splits each candidate's full name at each
# blank space, then takes just the candidate's first name
elections["First Name"] = elections["Candidate"].str.split().str[0]
elections.head(5)
```

	Year	Candidate	Party	Popular vote	Result	%	First Name
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.210122	Andrew
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.789878	John
2	1828	Andrew Jackson	Democratic	642806	win	56.203927	Andrew
3	1828	John Quincy Adams	National Republican	500897	loss	43.796073	John
4	1832	Andrew Jackson	Democratic	702735	win	54.574789	Andrew

```
# Here, we'll only consider `babynames` data from 2022
babynames_2022 = babynames[babynames["Year"]==2022]
babynames_2022.head()
```

	State	Sex	Year	Name	Count	First Letter
405695	CA	M	2022	Deandre	18	D
237964	CA	F	2022	Leandra	10	L
404916	CA	M	2022	Leandro	99	L
405892	CA	M	2022	Andreas	14	A
235927	CA	F	2022	Andrea	322	A

Now, we're ready to join the two tables. `pd.merge` is the **pandas** method used to join **DataFrames** together.

```
merged = pd.merge(left = elections, right = babynames_2022, \
                  left_on = "First Name", right_on = "Name")
merged.head()
# Notice that pandas automatically specifies `Year_x` and `Year_y`
# when both merged DataFrames have the same column name to avoid confusion

# Second option
# merged = elections.merge(right = babynames_2022, \
#                          left_on = "First Name", right_on = "Name")
```

	Year_x	Candidate	Party	Popular vote	Result	%	First Name	State	Sex	Year_y	Name	Co
0	1824	Andrew Jackson		Democratic-Republican		151271		loss		57.210122	Andrew	
1	1824	John Quincy Adams		Democratic-Republican		113142		win		42.789878	John	
2	1828	Andrew Jackson		Democratic		642806		win		56.203927	Andrew	
3	1828	John Quincy Adams		National Republican		500897		loss		43.796073	John	
4	1832	Andrew Jackson		Democratic		702735		win		54.574789	Andrew	

Let's take a closer look at the parameters:

- `left` and `right` parameters are used to specify the **DataFrames** to be joined.
- `left_on` and `right_on` parameters are assigned to the string names of the columns to be used when performing the join. These two **on** parameters tell **pandas** what values should act as pairing keys to determine which rows to merge across the **DataFrames**. We'll talk more about this idea of a pairing key next lecture.

## 4.6 Parting Note

Congratulations! We finally tackled **pandas**. Don't worry if you are still not feeling very comfortable with it—you will have plenty of chances to practice over the next few weeks.

Next, we will get our hands dirty with some real-world datasets and use our **pandas** knowledge to conduct some exploratory data analysis.

## 5 Data Cleaning and EDA

```
import numpy as np
import pandas as pd

import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
plt.rcParams['figure.figsize'] = (12, 9)

sns.set()
sns.set_context('talk')
np.set_printoptions(threshold=20, precision=2, suppress=True)
pd.set_option('display.max_rows', 30)
pd.set_option('display.max_columns', None)
pd.set_option('display.precision', 2)
# This option stops scientific notation for pandas
pd.set_option('display.float_format', '{:.2f}'.format)

# Silence some spurious seaborn warnings
import warnings
warnings.filterwarnings("ignore", category=FutureWarning)
warnings.filterwarnings("ignore", category=UserWarning)
```

### Learning Outcomes

- Recognize common file formats
- Categorize data by its variable type
- Build awareness of issues with data faithfulness and develop targeted solutions

In the past few lectures, we've learned that **pandas** is a toolkit to restructure, modify, and explore a dataset. What we haven't yet touched on is *how* to make these data transformation decisions. When we receive a new set of data from the “real world,” how do we know what processing we should do to convert this data into a usable form?

**Data cleaning**, also called **data wrangling**, is the process of transforming raw data to facilitate subsequent analysis. It is often used to address issues like:

- Unclear structure or formatting
- Missing or corrupted values
- Unit conversions
- ...and so on

**Exploratory Data Analysis (EDA)** is the process of understanding a new dataset. It is an open-ended, informal analysis that involves familiarizing ourselves with the variables present in the data, discovering potential hypotheses, and identifying possible issues with the data. This last point can often motivate further data cleaning to address any problems with the dataset's format; because of this, EDA and data cleaning are often thought of as an “infinite loop,” with each process driving the other.

In this lecture, we will consider the key properties of data to consider when performing data cleaning and EDA. In doing so, we'll develop a “checklist” of sorts for you to consider when approaching a new dataset. Throughout this process, we'll build a deeper understanding of this early (but very important!) stage of the data science lifecycle.

## 5.1 Structure

We often prefer rectangular data for data analysis. Rectangular structures are easy to manipulate and analyze. A key element of data cleaning is about transforming data to be more rectangular.

There are two kinds of rectangular data: tables and matrices. Tables have named columns with different data types and are manipulated using data transformation languages. Matrices contain numeric data of the same type and are manipulated using linear algebra.

### 5.1.1 File Formats

There are many file types for storing structured data: TSV, JSON, XML, ASCII, SAS, etc. We'll only cover CSV, TSV, and JSON in lecture, but you'll likely encounter other formats as you work with different datasets. Reading documentation is your best bet for understanding how to process the multitude of different file types.

#### 5.1.1.1 CSV

CSVs, which stand for **Comma-Separated Values**, are a common tabular data format. In the past two **pandas** lectures, we briefly touched on the idea of file format: the way data is encoded in a file for storage. Specifically, our **elections** and **babynames** datasets were stored and loaded as CSVs:

```
pd.read_csv("data/elections.csv").head(5)
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.21
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.79
2	1828	Andrew Jackson	Democratic	642806	win	56.20
3	1828	John Quincy Adams	National Republican	500897	loss	43.80
4	1832	Andrew Jackson	Democratic	702735	win	54.57

To better understand the properties of a CSV, let's take a look at the first few rows of the raw data file to see what it looks like before being loaded into a `DataFrame`. We'll use the `repr()` function to return the raw string with its special characters:

```
with open("data/elections.csv", "r") as table:
    i = 0
    for row in table:
        print(repr(row))
        i += 1
        if i > 3:
            break
```

```
'Year,Candidate,Party,Popular vote,Result,%\n'
'1824,Andrew Jackson,Democratic-Republican,151271,loss,57.21012204\n'
'1824,John Quincy Adams,Democratic-Republican,113142,win,42.78987796\n'
'1828,Andrew Jackson,Democratic,642806,win,56.20392707\n'
```

Each row, or **record**, in the data is delimited by a newline `\n`. Each column, or **field**, in the data is delimited by a comma `,` (hence, comma-separated!).

### 5.1.1.2 TSV

Another common file type is **TSV (Tab-Separated Values)**. In a TSV, records are still delimited by a newline `\n`, while fields are delimited by `\t` tab character.

Let's check out the first few rows of the raw TSV file. Again, we'll use the `repr()` function so that `print` shows the special characters.



```
with open("data/elections.txt", "r") as table:
    i = 0
    for row in table:
        print(repr(row))
        i += 1
        if i > 3:
            break
```

```
'i>Year\tCandidate\tParty\tPopular vote\tResult\t%\n'
'1824\tAndrew Jackson\tDemocratic-Republican\t151271\tloss\t57.21012204\n'
'1824\tJohn Quincy Adams\tDemocratic-Republican\t113142\twin\t42.78987796\n'
'1828\tAndrew Jackson\tDemocratic\t642806\twin\t56.20392707\n'
```

TSVs can be loaded into `pandas` using `pd.read_csv`. We'll need to specify the **delimiter** with parameter `sep='\t'` ([documentation](#)).

```
pd.read_csv("data/elections.txt", sep='\t').head(3)
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.21
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.79
2	1828	Andrew Jackson	Democratic	642806	win	56.20

An issue with CSVs and TSVs comes up whenever there are commas or tabs within the records. How does `pandas` differentiate between a comma delimiter vs. a comma within the field itself, for example 8,900? To remedy this, check out the [quotechar](#) parameter.

### 5.1.1.3 JSON

**JSON (JavaScript Object Notation)** files behave similarly to Python dictionaries. A raw JSON is shown below.

```
with open("data/elections.json", "r") as table:
    i = 0
    for row in table:
        print(row)
        i += 1
        if i > 8:
            break
```

```
[
{
  "Year": 1824,
  "Candidate": "Andrew Jackson",
  "Party": "Democratic-Republican",
  "Popular vote": 151271,
  "Result": "loss",
  "%": 57.21012204
},
```

JSON files can be loaded into `pandas` using `pd.read_json`.

```
pd.read_json('data/elections.json').head(3)
```

	Year	Candidate	Party	Popular vote	Result	%
0	1824	Andrew Jackson	Democratic-Republican	151271	loss	57.21
1	1824	John Quincy Adams	Democratic-Republican	113142	win	42.79
2	1828	Andrew Jackson	Democratic	642806	win	56.20

#### 5.1.1.3.1 EDA with JSON: Berkeley COVID-19 Data

The City of Berkeley Open Data [website](#) has a dataset with COVID-19 Confirmed Cases among Berkeley residents by date. Let's download the file and save it as a JSON (note the source URL file type is also a JSON). In the interest of reproducible data science, we will download the data programatically. We have defined some helper functions in the [ds100\\_utils.py](#) file that we can reuse these helper functions in many different notebooks.

```
from ds100_utils import fetch_and_cache

covid_file = fetch_and_cache(
    "https://data.cityofberkeley.info/api/views/xn6j-b766/rows.json?accessType=DOWNLOAD",
    "confirmed-cases.json",
```

```
force=False)
covid_file      # a file path wrapper object
```

Using cached version that was downloaded (UTC): Mon Jan 20 20:49:53 2025

```
WindowsPath('data/confirmed-cases.json')
```

#### 5.1.1.3.1.1 File Size

Let's start our analysis by getting a rough estimate of the size of the dataset to inform the tools we use to view the data. For relatively small datasets, we can use a text editor or spreadsheet. For larger datasets, more programmatic exploration or distributed computing tools may be more fitting. Here we will use **Python** tools to probe the file.

Since there seem to be text files, let's investigate the number of lines, which often corresponds to the number of records

```
import os

print(covid_file, "is", os.path.getsize(covid_file) / 1e6, "MB")

with open(covid_file, "r") as f:
    print(covid_file, "is", sum(1 for l in f), "lines.")
```

```
data\confirmed-cases.json is 0.117476 MB
data\confirmed-cases.json is 1110 lines.
```

#### 5.1.1.3.1.2 Unix Commands

As part of the EDA workflow, Unix commands can come in very handy. In fact, there's an entire book called [“Data Science at the Command Line”](#) that explores this idea in depth! In Jupyter/IPython, you can prefix lines with **!** to execute arbitrary Unix commands, and within those lines, you can refer to Python variables and expressions with the syntax **{expr}**.

Here, we use the **ls** command to list files, using the **-lh** flags, which request “long format with information in human-readable form.” We also use the **wc** command for “word count,” but with the **-l** flag, which asks for line counts instead of words.

These two give us the same information as the code above, albeit in a slightly different form:

```
!ls -lh {covid_file}
!wc -l {covid_file}
```

```
-rw-r--r-- 1 conan 197609 115K Jan 20 20:49 data\confirmed-cases.json
1109 data\confirmed-cases.json
```

#### 5.1.1.3.1.3 File Contents

Let's explore the data format using Python.

```
with open(covid_file, "r") as f:
    for i, row in enumerate(f):
        print(repr(row)) # print raw strings
        if i >= 4: break
```

```
'{\n'
'  "meta" : {\n'
'    "view" : {\n'
'      "id" : "xn6j-b766",\n'
'      "name" : "COVID-19 Confirmed Cases",\n'
```

We can use the `head` Unix command (which is where `pandas`' `head` method comes from!) to see the first few lines of the file:

```
!head -5 {covid_file}
```

```
{
  "meta" : {
    "view" : {
      "id" : "xn6j-b766",
      "name" : "COVID-19 Confirmed Cases",
```

In order to load the JSON file into `pandas`, Let's first do some EDA with Python's `json` package to understand the particular structure of this JSON file so that we can decide what (if anything) to load into `pandas`. Python has relatively good support for JSON data since it closely matches the internal python object model. In the following cell we import the entire JSON datafile into a python dictionary using the `json` package.

```
import json

with open(covid_file, "rb") as f:
    covid_json = json.load(f)
```

The `covid_json` variable is now a dictionary encoding the data in the file:

```
type(covid_json)
```

```
dict
```

We can examine what keys are in the top level JSON object by listing out the keys.

```
covid_json.keys()
```

```
dict_keys(['meta', 'data'])
```

**Observation:** The JSON dictionary contains a `meta` key which likely refers to metadata (data about the data). Metadata is often maintained with the data and can be a good source of additional information.

We can investigate the metadata further by examining the keys associated with the metadata.

```
covid_json['meta'].keys()
```

```
dict_keys(['view'])
```

The `meta` key contains another dictionary called `view`. This likely refers to metadata about a particular “view” of some underlying database. We will learn more about views when we study SQL later in the class.

```
covid_json['meta']['view'].keys()
```

```
dict_keys(['id', 'name', 'assetType', 'attribution', 'averageRating', 'category', 'createdAt'])
```

Notice that this is a nested/recursive data structure. As we dig deeper we reveal more and more keys and the corresponding data:

```

meta
|-> data
| ... (haven't explored yet)
|-> view
| -> id
| -> name
| -> attribution
...
| -> description
...
| -> columns
...

```

There is a key called `description` in the `view` sub dictionary. This likely contains a description of the data:

```
print(covid_json['meta']['view']['description'])
```

Counts of confirmed COVID-19 cases among Berkeley residents by date.

#### 5.1.1.3.1.4 Examining the Data Field for Records

We can look at a few entries in the `data` field. This is what we'll load into `pandas`.

```

for i in range(3):
    print(f"{i:03} | {covid_json['data'][i]}")

```

```

000 | ['row-kzbg.v7my-c3y2', '00000000-0000-0000-0405-CB14DE51DAA7', 0, 1643733903, None, 1643733903]
001 | ['row-jkyx_9u4r-h2yw', '00000000-0000-0000-F806-86D0DBE0E17F', 0, 1643733903, None, 1643733903]
002 | ['row-qifg_4aug-y3ym', '00000000-0000-0000-2DCE-4D1872F9B216', 0, 1643733903, None, 1643733903]

```

Observations:

- These look like equal-length records, so maybe `data` is a table!
- But what do each of values in the record mean? Where can we find column headers?

For that, we'll need the `columns` key in the metadata dictionary. This returns a list:

```
type(covid_json['meta']['view']['columns'])
```

```
list
```

#### 5.1.1.3.1.5 Summary of exploring the JSON file

1. The above **metadata** tells us a lot about the columns in the data including column names, potential data anomalies, and a basic statistic.
2. Because of its non-tabular structure, JSON makes it easier (than CSV) to create **self-documenting data**, meaning that information about the data is stored in the same file as the data.
3. Self-documenting data can be helpful since it maintains its own description and these descriptions are more likely to be updated as data changes.

#### 5.1.1.3.1.6 Loading COVID Data into pandas

Finally, let's load the data (not the metadata) into a **pandas DataFrame**. In the following block of code we:

1. Translate the JSON records into a **DataFrame**:
  - fields: `covid_json['meta']['view']['columns']`
  - records: `covid_json['data']`
2. Remove columns that have no metadata description. This would be a bad idea in general, but here we remove these columns since the above analysis suggests they are unlikely to contain useful information.
3. Examine the **tail** of the table.

```
# Load the data from JSON and assign column titles
covid = pd.DataFrame(
    covid_json['data'],
    columns=[c['name'] for c in covid_json['meta']['view']['columns']])

covid.tail()
```

	sid	id	position	created_at	created_meta	updated_at	updated_meta	meta	Date	New Cases
699	row-49b6_x8zv.gyum			00000000-0000-0000-A18C-9174A6D05774			0	1643733903	None	
700	row-gs55-p5em.y4v9			00000000-0000-0000-F41D-5724AEABB4D6			0	1643733903	None	
701	row-3pyj.tf95-qu67			00000000-0000-0000-BEE3-B0188D2518BD			0	1643733903	None	
702	row-cgnd.8syv.jvjn			00000000-0000-0000-C318-63CF75F7F740			0	1643733903	None	
703	row-qyvv_24x6-237y			00000000-0000-0000-FE92-9789FED3AA20			0	1643733903	None	

### 5.1.2 Variable Types

Variables are columns. A variable is a measurement of a particular concept. Variables have two common properties: data type/storage type and variable type/feature type. The data type of a variable indicates how each variable value is stored in memory (integer, floating point, boolean, etc.) and affects which **pandas** functions are used. The variable type is a conceptualized measurement of information (and therefore indicates what values a variable can take on). Variable type is identified through expert knowledge, exploring the data itself, or consulting the data codebook. The variable type affects how one visualizes and interprets the data. In this class, “variable types” are conceptual.

After loading data into a file, it’s a good idea to take the time to understand what pieces of information are encoded in the dataset. In particular, we want to identify what variable types are present in our data. Broadly speaking, we can categorize variables into one of two overarching types.

**Quantitative variables** describe some numeric quantity or amount. Some examples include weights, GPA, CO2 concentrations, someone’s age, or the number of siblings they have.

**Qualitative variables**, also known as **categorical variables**, describe data that isn’t measuring some quantity or amount. The sub-categories of categorical data are:

- **Ordinal qualitative variables:** categories with ordered levels. Specifically, ordinal variables are those where the difference between levels has no consistent, quantifiable meaning. Some examples include levels of education (high school, undergrad, grad, etc.), income bracket (low, medium, high), or Yelp rating.
- **Nominal qualitative variables:** categories with no specific order. For example, someone’s political affiliation or Cal ID number.



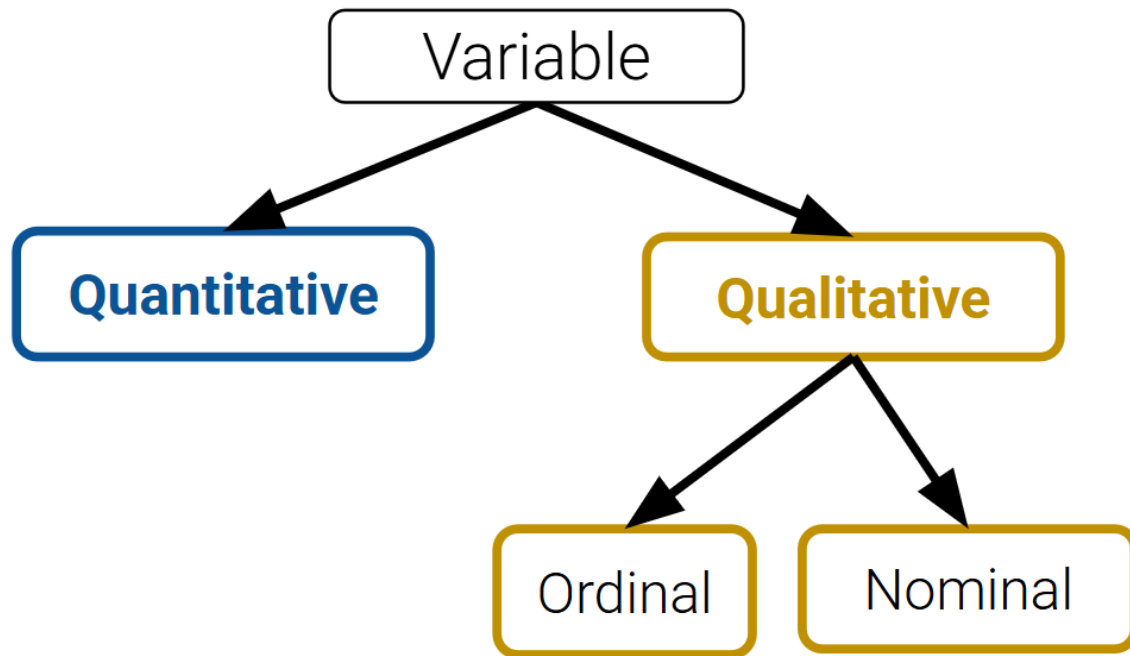


Figure 5.1: Classification of variable types

Note that many variables don't sit neatly in just one of these categories. Qualitative variables could have numeric levels, and conversely, quantitative variables could be stored as strings.

## 5.2 Granularity and Temporality

After understanding the structure of the dataset, the next task is to determine what exactly the data represents. We'll do so by considering the data's granularity and temporality.

### 5.2.1 Granularity

The **granularity** of a dataset is what a single row represents. You can also think of it as the level of detail included in the data. To determine the data's granularity, ask: what does each row in the dataset represent? Fine-grained data contains a high level of detail, with a single row representing a small individual unit. For example, each record may represent one person. Coarse-grained data is encoded such that a single row represents a large individual unit – for example, each record may represent a group of people.

## 5.2.2 Temporality

The **temporality** of a dataset describes the periodicity over which the data was collected as well as when the data was most recently collected or updated.

Time and date fields of a dataset could represent a few things:

1. when the “event” happened
2. when the data was collected, or when it was entered into the system
3. when the data was copied into the database

To fully understand the temporality of the data, it also may be necessary to standardize time zones or inspect recurring time-based trends in the data (do patterns recur in 24-hour periods? Over the course of a month? Seasonally?). The convention for standardizing time is the Coordinated Universal Time (UTC), an international time standard measured at 0 degrees latitude that stays consistent throughout the year (no daylight savings). We can represent Berkeley’s time zone, Pacific Standard Time (PST), as UTC-7 (with daylight savings).

### 5.2.2.1 Temporality with pandas’ dt accessors

Let’s briefly look at how we can use pandas’ dt accessors to work with dates/times in a dataset using the dataset you’ll see in Lab 3: the Berkeley PD Calls for Service dataset.

```
calls = pd.read_csv("data/Berkeley_PD_-_Calls_for_Service.csv")
calls.head()
```

	CASENO	OFFENSE	EVENTDT	EVENTTM	CVLEGEND	CVDOW	InDbDate	Block_Location
0	21014296	THEFT MISD. (UNDER \$950)	04/01/2021	12:00:00 AM	10:58		LARCENY	
1	21014391	THEFT MISD. (UNDER \$950)	04/01/2021	12:00:00 AM	10:38		LARCENY	
2	21090494	THEFT MISD. (UNDER \$950)	04/19/2021	12:00:00 AM	12:15		LARCENY	
3	21090204	THEFT FELONY (OVER \$950)	02/13/2021	12:00:00 AM	17:00		LARCENY	
4	21090179	BURGLARY AUTO	02/08/2021	12:00:00 AM	6:20		BURGLARY - VI	

Looks like there are three columns with dates/times: **EVENTDT**, **EVENTTM**, and **InDbDate**.

Most likely, **EVENTDT** stands for the date when the event took place, **EVENTTM** stands for the time of day the event took place (in 24-hr format), and **InDbDate** is the date this call is recorded onto the database.

If we check the data type of these columns, we will see they are stored as strings. We can convert them to **datetime** objects using pandas **to\_datetime** function.

```
calls["EVENTDT"] = pd.to_datetime(calls["EVENTDT"])
calls.head()
```

	CASENO	OFFENSE	EVENTDT	EVENTTM	CVLEGEND	CVDOW	InDbDate	Block_Location
0	21014296	THEFT MISD. (UNDER \$950)	2021-04-01	10:58		LARCENY		4
1	21014391	THEFT MISD. (UNDER \$950)	2021-04-01	10:38		LARCENY		4
2	21090494	THEFT MISD. (UNDER \$950)	2021-04-19	12:15		LARCENY		1
3	21090204	THEFT FELONY (OVER \$950)	2021-02-13	17:00		LARCENY		6
4	21090179	BURGLARY AUTO	2021-02-08	6:20		BURGLARY - VEHICLE		1

Now, we can use the `dt` accessor on this column.

We can get the month:

```
calls["EVENTDT"].dt.month.head()
```

```
0    4
1    4
2    4
3    2
4    2
Name: EVENTDT, dtype: int32
```

Which day of the week the date is on:

```
calls["EVENTDT"].dt.dayofweek.head()
```

```
0    3
1    3
2    0
3    5
4    0
Name: EVENTDT, dtype: int32
```

Check the minimum values to see if there are any suspicious-looking, 70s dates:

```
calls.sort_values("EVENTDT").head()
```

	CASENO	OFFENSE	EVENTDT	EVENTTM	CVLEGEND	CVDOW	InDbDate	Block_Location
2513	20057398	BURGLARY COMMERCIAL		2020-12-17	16:05		BURGLARY - COMMERCIAL	
624	20057207	ASSAULT/BATTERY MISD.		2020-12-17	16:50		ASSAULT	
154	20092214	THEFT FROM AUTO		2020-12-17	18:30		LARCENY - FROM VEHICLE	
659	20057324	THEFT MISD. (UNDER \$950)		2020-12-17	15:44		LARCENY	
993	20057573	BURGLARY RESIDENTIAL		2020-12-17	22:15		BURGLARY - RESIDENTIAL	

Doesn't look like it! We are good!

We can also do many things with the `dt` accessor like switching time zones and converting time back to UNIX/POSIX time. Check out the documentation on [.dt accessor](#) and [time series/date functionality](#).

## 5.3 Faithfulness

At this stage in our data cleaning and EDA workflow, we've achieved quite a lot: we've identified how our data is structured, come to terms with what information it encodes, and gained insight as to how it was generated. Throughout this process, we should always recall the original intent of our work in Data Science – to use data to better understand and model the real world. To achieve this goal, we need to ensure that the data we use is faithful to reality; that is, that our data accurately captures the “real world.”

Data used in research or industry is often “messy” – there may be errors or inaccuracies that impact the faithfulness of the dataset. Signs that data may not be faithful include:

- Unrealistic or “incorrect” values, such as negative counts, locations that don't exist, or dates set in the future
- Violations of obvious dependencies, like an age that does not match a birthday
- Clear signs that data was entered by hand, which can lead to spelling errors or fields that are incorrectly shifted
- Signs of data falsification, such as fake email addresses or repeated use of the same names
- Duplicated records or fields containing the same information
- Truncated data, e.g. Microsoft Excel would limit the number of rows to 65536 and the number of columns to 255

We often solve some of these more common issues in the following ways:

- Spelling errors: apply corrections or drop records that aren't in a dictionary
- Time zone inconsistencies: convert to a common time zone (e.g. UTC)
- Duplicated records or fields: identify and eliminate duplicates (using primary keys)
- Unspecified or inconsistent units: infer the units and check that values are in reasonable ranges in the data

### 5.3.1 Missing Values

Another common issue encountered with real-world datasets is that of missing data. One strategy to resolve this is to simply drop any records with missing values from the dataset. This does, however, introduce the risk of inducing biases – it is possible that the missing or corrupt records may be systemically related to some feature of interest in the data. Another solution is to keep the data as NaN values.

A third method to address missing data is to perform **imputation**: infer the missing values using other data available in the dataset. There is a wide variety of imputation techniques that can be implemented; some of the most common are listed below.

- Average imputation: replace missing values with the average value for that field
- Hot deck imputation: replace missing values with some random value
- Regression imputation: develop a model to predict missing values and replace with the predicted value from the model.
- Multiple imputation: replace missing values with multiple random values

Regardless of the strategy used to deal with missing data, we should think carefully about *why* particular records or fields may be missing – this can help inform whether or not the absence of these values is significant or meaningful.

## 5.4 EDA Demo 1: Tuberculosis in the United States

Now, let's walk through the data-cleaning and EDA workflow to see what can we learn about the presence of Tuberculosis in the United States!

We will examine the data included in the [original CDC article](#) published in 2021.

### 5.4.1 CSVs and Field Names

Suppose Table 1 was saved as a CSV file located in `data/cdc_tuberculosis.csv`.

We can then explore the CSV (which is a text file, and does not contain binary-encoded data) in many ways: 1. Using a text editor like emacs, vim, VSCode, etc. 2. Opening the CSV directly in DataHub (read-only), Excel, Google Sheets, etc. 3. The Python file object 4. `pandas`, using `pd.read_csv()`

To try out options 1 and 2, you can view or download the Tuberculosis from the [lecture demo notebook](#) under the `data` folder in the left hand menu. Notice how the CSV file is a type of **rectangular data (i.e., tabular data) stored as comma-separated values**.

Next, let's try out option 3 using the Python file object. We'll look at the first four lines:

```
with open("data/cdc_tuberculosis.csv", "r") as f:
    i = 0
    for row in f:
        print(row)
        i += 1
        if i > 3:
            break
```

,No. of TB cases,,

U.S. jurisdiction,2019,2020,2021

Total,"8,900","7,173","7,860"

Alabama,87,72,92

Whoa, why are there blank lines interspaced between the lines of the CSV?

You may recall that all line breaks in text files are encoded as the special newline character `\n`. Python's `print()` prints each string (including the newline), and an additional newline on top of that.

If you're curious, we can use the `repr()` function to return the raw string with all special characters:

```
with open("data/cdc_tuberculosis.csv", "r") as f:
    i = 0
    for row in f:
        print(repr(row)) # print raw strings
        i += 1
        if i > 3:
            break
```

',No. of TB cases,,\n'

'U.S. jurisdiction,2019,2020,2021\n'

'Total,"8,900","7,173","7,860"\n'

'Alabama,87,72,92\n'

Finally, let's try option 4 and use the tried-and-true Data 100 approach: `pandas`.

```
tb_df = pd.read_csv("data/cdc_tuberculosis.csv")
tb_df.head()
```

	Unnamed: 0	No. of TB cases	Unnamed: 2	Unnamed: 3
0	U.S. jurisdiction	2019	2020	2021
1	Total	8,900	7,173	7,860
2	Alabama	87	72	92
3	Alaska	58	58	58
4	Arizona	183	136	129

You may notice some strange things about this table: what’s up with the “Unnamed” column names and the first row?

Congratulations — you’re ready to wrangle your data! Because of how things are stored, we’ll need to clean the data a bit to name our columns better.

A reasonable first step is to identify the row with the right header. The `pd.read_csv()` function ([documentation](#)) has the convenient `header` parameter that we can set to use the elements in row 1 as the appropriate columns:

```
tb_df = pd.read_csv("data/cdc_tuberculosis.csv", header=1) # row index
tb_df.head(5)
```

	U.S. jurisdiction	2019	2020	2021
0	Total	8,900	7,173	7,860
1	Alabama	87	72	92
2	Alaska	58	58	58
3	Arizona	183	136	129
4	Arkansas	64	59	69

## 5.4.2 Record Granularity

You might already be wondering: what’s up with that first record?

Row 0 is what we call a **rollup record**, or summary record. It’s often useful when displaying tables to humans. The **granularity** of record 0 (Totals) vs the rest of the records (States) is different.

Okay, EDA step two. How was the rollup record aggregated?

Let's check if Total TB cases is the sum of all state TB cases. If we sum over all rows, we should get **2x** the total cases in each of our TB cases by year (why do you think this is?).

```
tb_df.sum(axis=0)
```

```
U.S. jurisdiction    TotalAlabamaAlaskaArizonaArkansasCaliforniaCol...
2019                8,9008758183642,111666718245583029973261085237...
2020                7,1737258136591,706525417194122219282169239376...
2021                7,8609258129691,750585443194992281064255127494...
dtype: object
```

Whoa, what's going on with the TB cases in 2019, 2020, and 2021? Check out the column types:

```
tb_df.dtypes
```

```
U.S. jurisdiction    object
2019                object
2020                object
2021                object
dtype: object
```

Since there are commas in the values for TB cases, the numbers are read as the **object** datatype, or **storage type** (close to the Python string datatype), so **pandas** is concatenating strings instead of adding integers (recall that Python can “sum”, or concatenate, strings together: “data” + “100” evaluates to “data100”).

Fortunately `read_csv` also has a `thousands` parameter ([documentation](#)):

```
# improve readability: chaining method calls with outer parentheses/line breaks
tb_df = (
    pd.read_csv("data/cdc_tuberculosis.csv", header=1, thousands=',')
)
tb_df.head(5)
```

	U.S. jurisdiction	2019	2020	2021
0	Total	8900	7173	7860
1	Alabama	87	72	92
2	Alaska	58	58	58



	U.S. jurisdiction	2019	2020	2021
3	Arizona	183	136	129
4	Arkansas	64	59	69

```
tb_df.sum()
```

```
U.S. jurisdiction    TotalAlabamaAlaskaArizonaArkansasCaliforniaCol...
2019                                                         17800
2020                                                         14346
2021                                                         15720
dtype: object
```

The total TB cases look right. Phew!

Let's just look at the records with **state-level granularity**:

```
state_tb_df = tb_df[1:]
state_tb_df.head(5)
```

	U.S. jurisdiction	2019	2020	2021
1	Alabama	87	72	92
2	Alaska	58	58	58
3	Arizona	183	136	129
4	Arkansas	64	59	69
5	California	2111	1706	1750

### 5.4.3 Gather Census Data

U.S. Census population estimates [source](#) (2019), [source](#) (2020-2024).

Running the below cells cleans the data. There are a few new methods here:

- `df.convert_dtypes()` ([documentation](#)) conveniently converts all float dtypes into ints and is out of scope for the class.
- `df.drop_na()` ([documentation](#)) will be explained in more detail next time.

```
# 2010s census data
census_2010s_df = pd.read_csv("data/nst-est2019-01.csv", header=3, thousands=",")
census_2010s_df = (
    census_2010s_df
    .rename(columns={"Unnamed: 0": "Geographic Area"})
    .drop(columns=["Census", "Estimates Base"])
    .convert_dtypes() # "smart" converting of columns to int, use at your own risk
    .dropna() # we'll introduce this very soon
)
census_2010s_df['Geographic Area'] = census_2010s_df['Geographic Area'].str.strip('.')

# with pd.option_context('display.min_rows', 30): # shows more rows
#     display(census_2010s_df)

census_2010s_df.head(5)
```

	Geographic Area	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
0	United States	309321666	311556874	313830990	315993715	318301008	320635163	322941311			
1	Northeast	55380134	55604223	55775216	55901806	56006011	56034684	56042330			
2	Midwest	66974416	67157800	67336743	67560379	67745167	67860583	67987540			
3	South	114866680	116006522	117241208	118364400	119624037	120997341	122351760			
4	West	72100436	72788329	73477823	74167130	74925793	75742555	76559681			

Occasionally, you will want to modify code that you have imported. To reimport those modifications you can either use python's `importlib` library:

```
from importlib import reload
reload(utils)
```

or use `iPython` magic which will intelligently import code when files change:

```
%load_ext autoreload
%autoreload 2
```

```
# census 2020s data
census_2020s_df = pd.read_csv("data/NST-EST2024-POP.csv", header=3, thousands=",")
census_2020s_df = (
    census_2020s_df
    .drop(columns=["Unnamed: 1"])
    .rename(columns={"Unnamed: 0": "Geographic Area"})
)
```

```

.loc[:, "Geographic Area":"2024"] # ignore all the blank extra columns
.convert_dtypes()                  # "smart" converting of columns, use at your own risk
.dropna()                          # we'll introduce this next ti
)
census_2020s_df['Geographic Area'] = census_2020s_df['Geographic Area'].str.strip('.')
census_2020s_df.head(5)

```

		Geographic Area	2020	2021	2022	2023	2024
0	United States	331577720	332099760	334017321	336806231	340110988	
1	Northeast	57431458	57252533	57159597	57398303	57832935	
2	Midwest	68984258	68872831	68903297	69186401	69596584	
3	South	126476549	127368010	129037849	130893358	132665693	
4	West	78685455	78606386	78916578	79328169	80015776	

#### 5.4.4 Joining Data (Merging DataFrames)

Time to merge! Here we use the `DataFrame` method `df1.merge(right=df2, ...)` on `DataFrame` `df1` ([documentation](#)). Contrast this with the function `pd.merge(left=df1, right=df2, ...)` ([documentation](#)). Feel free to use either.

```

# merge TB DataFrame with two US census DataFrames
tb_census_df = (
    tb_df
    .merge(right=census_2010s_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area")
    .merge(right=census_2020s_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area")
)
tb_census_df.head(5)

```

	U.S. jurisdiction	2019_x	2020_x	2021_x	Geographic Area_x	2010	2011	2012	2013	2014	2015
0	Alabama	87	72	92	Alabama	4785437	4799069	4815588	4831144	4846700	4862256
1	Alaska	58	58	58	Alaska	713910	722128	730443	738758	747073	755388
2	Arizona	183	136	129	Arizona	6407172	6472643	6554978	6637144	6719310	6801476
3	Arkansas	64	59	69	Arkansas	2921964	2940667	2952164	2963661	2975158	2986655
4	California	2111	1706	1750	California	37319502	37638369	37948800	38258188	38567576	38876964

We're only interested in the population for the years 2019, 2020, and 2021, so let's select just those columns:

```
census_2019_df = census_2010s_df[['Geographic Area', '2019']]
census_2020_2021_df = census_2020s_df[['Geographic Area', '2020', '2021']]

display(tb_df.tail(2))
display(census_2019_df.tail(2))
display(census_2020_2021_df.tail(2))
```

	U.S. jurisdiction	2019	2020	2021
50	Wisconsin	51	35	66
51	Wyoming	1	0	3

	Geographic Area	2019
55	Wyoming	578759
57	Puerto Rico	3193694

	Geographic Area	2020	2021
55	Wyoming	577681	579636
57	Puerto Rico	3281590	3262711

All three dataframes have a column containing U.S. states, along with some other geographic areas. These columns are our **join keys**.

- Below, we use `df1.merge(right=df2, ...)` to carry out the merge ([documentation](#)).
- We could have alternatively used the function `pd.merge(left=df1, right=df2, ...)` ([documentation](#)).

```
# merge TB dataframe with two US census dataframes
tb_census_df = (
    tb_df
    .merge(right=census_2019_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area")
    .merge(right=census_2020_2021_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area")
)
tb_census_df.tail(2)
```

	U.S. jurisdiction	2019_x	2020_x	2021_x	Geographic Area_x	2019_y	Geographic Area_y	2020_y
49	Wisconsin	51	35	66	Wisconsin	5822434	Wisconsin	58
50	Wyoming	1	0	3	Wyoming	578759	Wyoming	57

To see what's going on with the duplicate columns, and the `_x` and `_y`, let's do the just the first merge:

```
tb_df.merge(right=census_2019_df,
            left_on="U.S. jurisdiction",
            right_on="Geographic Area").head()
```

	U.S. jurisdiction	2019_x	2020	2021	Geographic Area	2019_y
0	Alabama	87	72	92	Alabama	4903185
1	Alaska	58	58	58	Alaska	731545
2	Arizona	183	136	129	Arizona	7278717
3	Arkansas	64	59	69	Arkansas	3017804
4	California	2111	1706	1750	California	39512223

Notice that the columns containing the **join keys** have all been retained, and all contain the same values.

- Furthermore, notice that the duplicated columns are appended with `_x` and `_y` to keep the column names unique.
- In the TB case count data, column 2019 represents the number of TB cases in 2019, but in the Census data, column 2019 represents the U.S. population.

We can use the `suffixes` argument to modify the `_x` and `_y` defaults to our liking ([documentation](#)).

```
# Specify the suffixes to use for duplicated column names
tb_df.merge(right=census_2019_df,
            left_on="U.S. jurisdiction",
            right_on="Geographic Area",
            suffixes=('_cases', '_population')).head()
```

	U.S. jurisdiction	2019_cases	2020	2021	Geographic Area	2019_population
0	Alabama	87	72	92	Alabama	4903185
1	Alaska	58	58	58	Alaska	731545

	U.S. jurisdiction	2019_cases	2020	2021	Geographic Area	2019_population
2	Arizona	183	136	129	Arizona	7278717
3	Arkansas	64	59	69	Arkansas	3017804
4	California	2111	1706	1750	California	39512223

Notice the `_x` and `_y` have changed to `_cases` and `_population`, just like we specified.

Putting it all together, and dropping the duplicated `Geographic Area` columns:

```
# Redux: merge TB dataframe with two US census dataframes
tb_census_df = (
    tb_df

    .merge(right=census_2019_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area",
           suffixes=('_cases', '_population'))
    .drop(columns="Geographic Area")

    .merge(right=census_2020_2021_df,
           left_on="U.S. jurisdiction", right_on="Geographic Area",
           suffixes=('_cases', '_population'))
    .drop(columns="Geographic Area")

)
tb_census_df.tail(2)
```

	U.S. jurisdiction	2019_cases	2020_cases	2021_cases	2019_population	2020_population	2021_population
49	Wisconsin	51	35	66	5822434	5897375	588160
50	Wyoming	1	0	3	578759	577681	579636

### 5.4.5 Reproducing Data: Compute Incidence

Let's see if we can reproduce the original CDC numbers from our augmented dataset of TB case counts and state populations.

- Recall that the nationwide TB incidence was **2.7 in 2019**, **2.2 in 2020**, and **2.4 in 2021**.
- Along the way, we'll also compute state-level incidence.

From the [CDC report](#): TB incidence is computed as “Cases per 100,000 persons using mid-year population estimates from the U.S. Census Bureau.”

Let’s start with a simpler question: What is the per person incidence?

- In other words, what is the probability that a randomly selected person in the population had TB within a given year?

$$\text{TB incidence per person} = \frac{\# \text{ TB cases in population}}{\text{Total population size}}$$

Let’s calculate per person incidence for 2019:

```
# Calculate per person incidence for 2019
tb_census_df["per person incidence 2019"] = (
    tb_census_df["2019_cases"]/tb_census_df["2019_population"]
)
tb_census_df
```

	U.S. jurisdiction	2019_cases	2020_cases	2021_cases	2019_population	2020_population	2021_population
0	Alabama	87	72	92	4903185	5033094	504919
1	Alaska	58	58	58	731545	733017	734420
2	Arizona	183	136	129	7278717	7187135	727407
3	Arkansas	64	59	69	3017804	3014546	302687
4	California	2111	1706	1750	39512223	39521958	391425
...	...	...	...	...	...	...	...
46	Virginia	191	169	161	8535519	8637615	865891
47	Washington	221	163	199	7614893	7727209	774376
48	West Virginia	9	13	7	1792147	1791646	178561
49	Wisconsin	51	35	66	5822434	5897375	588160
50	Wyoming	1	0	3	578759	577681	579636

TB is really rare in the United States, so per person TB incidence is really low, as expected.

- But, if we were to consider 100,000 people, the probability of seeing a TB case is higher.
- In fact, it would be 100,000 times higher!

$$\text{TB incidence per 100,000} = 100,000 * \text{TB incidence per person}$$

```
# To help read bigger numbers in Python, you can use _ to separate thousands,
# akin to using commas. 100_000 is the same as writing 100000, but more readable.
tb_census_df["per 100k incidence 2019"] = (
    100_000 * tb_census_df["per person incidence 2019"]
)
tb_census_df
```

	U.S. jurisdiction	2019_cases	2020_cases	2021_cases	2019_population	2020_population	2021_population
0	Alabama	87	72	92	4903185	5033094	504919
1	Alaska	58	58	58	731545	733017	734420
2	Arizona	183	136	129	7278717	7187135	727407
3	Arkansas	64	59	69	3017804	3014546	302687
4	California	2111	1706	1750	39512223	39521958	391425
...	...	...	...	...	...	...	...
46	Virginia	191	169	161	8535519	8637615	865891
47	Washington	221	163	199	7614893	7727209	774376
48	West Virginia	9	13	7	1792147	1791646	178561
49	Wisconsin	51	35	66	5822434	5897375	588160
50	Wyoming	1	0	3	578759	577681	579636

Now we're seeing more human-readable values.

- For example, there 5.3 tuberculosis cases for every 100,000 California residents in 2019.

To wrap up this exercise, let's calculate the nationwide incidence of TB in 2019.

```
# Recall that the CDC reported an incidence of 2.7 per 100,000 in 2019.
tot_tb_cases_50_states = tb_census_df["2019_cases"].sum()
tot_pop_50_states = tb_census_df["2019_population"].sum()
tb_per_100k_50_states = 100_000 * tot_tb_cases_50_states / tot_pop_50_states
tb_per_100k_50_states
```

```
np.float64(2.7114346007625656)
```

We can use a `for` loop to compute the incidence for 2019, 2020, and 2021.

- You'll notice that we get the same numbers reported by the CDC!



```
# f strings (f"...") are a handy way to pass in variables to strings.
for year in [2019, 2020, 2021]:
    tot_tb_cases_50_states = tb_census_df[f"{year}_cases"].sum()
    tot_pop_50_states = tb_census_df[f"{year}_population"].sum()
    tb_per_100k_50_states = 100_000 * tot_tb_cases_50_states / tot_pop_50_states
    print(tb_per_100k_50_states)
```

```
2.7114346007625656
2.163293721906285
2.366758711298075
```

## 5.5 EDA Demo 2: Mauna Loa CO2 Data – A Lesson in Data Faithfulness

[Mauna Loa Observatory](#) has been monitoring CO2 concentrations since 1958.

```
co2_file = "data/co2_mm_mlo.txt"
```

Let's do some **EDA**!!

### 5.5.1 Reading this file into Pandas?

Let's instead check out this .txt file. Some questions to keep in mind: Do we trust this file extension? What structure is it?

Lines 71-78 (inclusive) are shown below:

line number		file contents						
71		#		decimal	average	interpolated	trend	#days
72		#		date			(season corr)	
73		1958	3	1958.208	315.71	315.71	314.62	-1
74		1958	4	1958.292	317.45	317.45	315.29	-1
75		1958	5	1958.375	317.50	317.50	314.71	-1
76		1958	6	1958.458	-99.99	317.10	314.85	-1
77		1958	7	1958.542	315.86	315.86	314.98	-1
78		1958	8	1958.625	314.93	314.93	315.94	-1

Notice how:

- The values are separated by white space, possibly tabs.
- The data line up down the rows. For example, the month appears in 7th to 8th position of each line.
- The 71st and 72nd lines in the file contain column headings split over two lines.

We can use `read_csv` to read the data into a **pandas DataFrame**, and we provide several arguments to specify that the separators are white space, there is no header (**we will set our own column names**), and to skip the first 72 rows of the file.

```
co2 = pd.read_csv(
    co2_file, header = None, skiprows = 72,
    sep = r'\s+'          #delimiter for continuous whitespace (stay tuned for regex next lecture)
)
co2.head()
```

			0	1	2	3	4	5	6
0	1958	3	1958.21	315.71	315.71	314.62	-1		
1	1958	4	1958.29	317.45	317.45	315.29	-1		
2	1958	5	1958.38	317.50	317.50	314.71	-1		
3	1958	6	1958.46	-99.99	317.10	314.85	-1		
4	1958	7	1958.54	315.86	315.86	314.98	-1		

Congratulations! You've wrangled the data!

...But our columns aren't named. **We need to do more EDA.**

## 5.5.2 Exploring Variable Feature Types

The NOAA [webpage](#) might have some useful tidbits (in this case it doesn't).

Using this information, we'll rerun `pd.read_csv`, but this time with some **custom column names**.

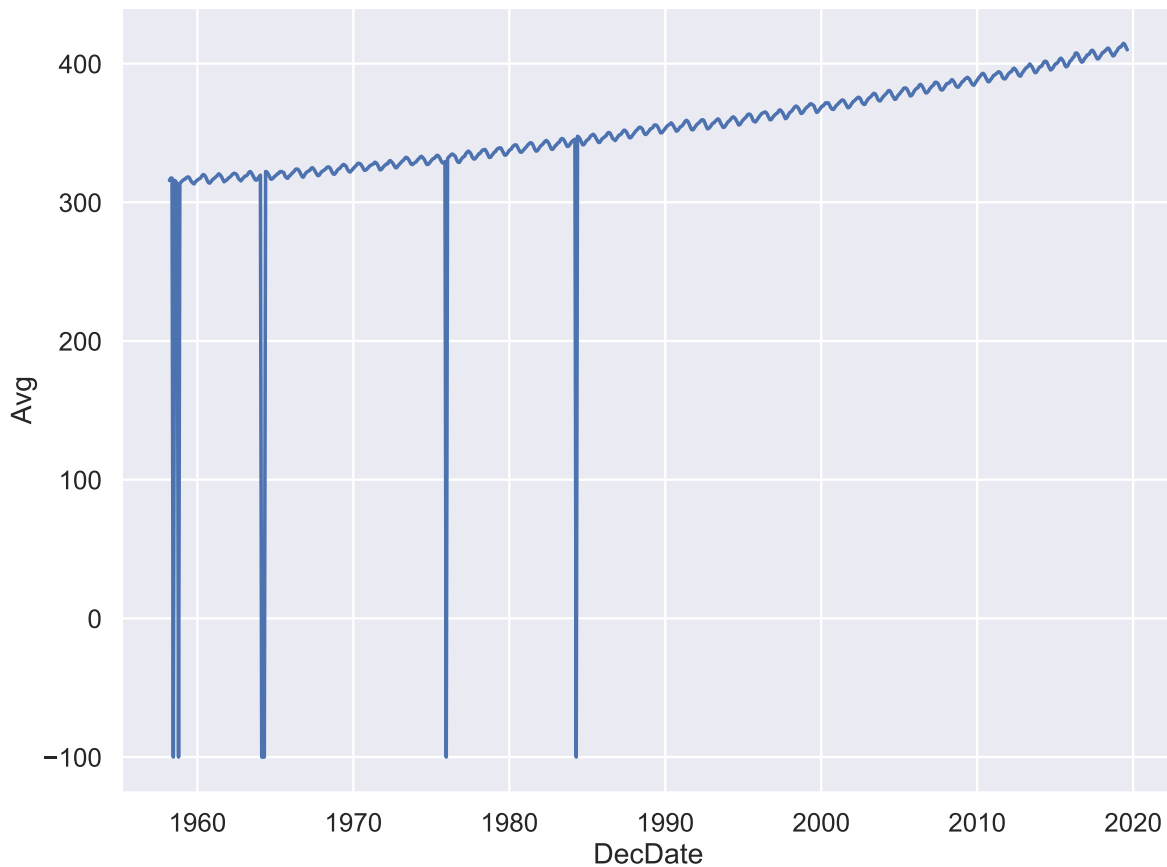
```
co2 = pd.read_csv(
    co2_file, header = None, skiprows = 72,
    sep = r'\s+', #regex for continuous whitespace (next lecture)
    names = ['Yr', 'Mo', 'DecDate', 'Avg', 'Int', 'Trend', 'Days']
)
co2.head()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
0	1958	3	1958.21	315.71	315.71	314.62	-1
1	1958	4	1958.29	317.45	317.45	315.29	-1
2	1958	5	1958.38	317.50	317.50	314.71	-1
3	1958	6	1958.46	-99.99	317.10	314.85	-1
4	1958	7	1958.54	315.86	315.86	314.98	-1

### 5.5.3 Visualizing CO2

Scientific studies tend to have very clean data, right...? Let's jump right in and make a time series plot of CO2 monthly averages.

```
sns.lineplot(x='DecDate', y='Avg', data=co2);
```



The code above uses the **seaborn** plotting library (abbreviated **sns**). We will cover this in the Visualization lecture, but now you don't need to worry about how it works!

Yikes! Plotting the data uncovered a problem. The sharp vertical lines suggest that we have some **missing values**. What happened here?

```
co2.head()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
0	1958	3	1958.21	315.71	315.71	314.62	-1
1	1958	4	1958.29	317.45	317.45	315.29	-1
2	1958	5	1958.38	317.50	317.50	314.71	-1
3	1958	6	1958.46	-99.99	317.10	314.85	-1
4	1958	7	1958.54	315.86	315.86	314.98	-1

```
co2.tail()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
733	2019	4	2019.29	413.32	413.32	410.49	26
734	2019	5	2019.38	414.66	414.66	411.20	28
735	2019	6	2019.46	413.92	413.92	411.58	27
736	2019	7	2019.54	411.77	411.77	411.43	23
737	2019	8	2019.62	409.95	409.95	411.84	29

Some data have unusual values like -1 and -99.99.

Let's check the description at the top of the file again.

- -1 signifies a missing value for the number of days **Days** the equipment was in operation that month.
- -99.99 denotes a missing monthly average **Avg**

How can we fix this? First, let's explore other aspects of our data. Understanding our data will help us decide what to do with the missing values.

#### 5.5.4 Sanity Checks: Reasoning about the data

First, we consider the shape of the data. How many rows should we have?

- If chronological order, we should have one record per month.
- Data from March 1958 to August 2019.
- We should have  $12 \times (2019 - 1957) - 2 - 4 = 738$  records.

```
co2.shape
```

```
(738, 7)
```

Nice!! The number of rows (i.e. records) match our expectations.

Let's now check the quality of each feature.

### 5.5.5 Understanding Missing Value 1: Days

**Days** is a time field, so let's analyze other time fields to see if there is an explanation for missing values of days of operation.

Let's start with **months**, **Mo**.

Are we missing any records? The number of months should have 62 or 61 instances (March 1957-August 2019).

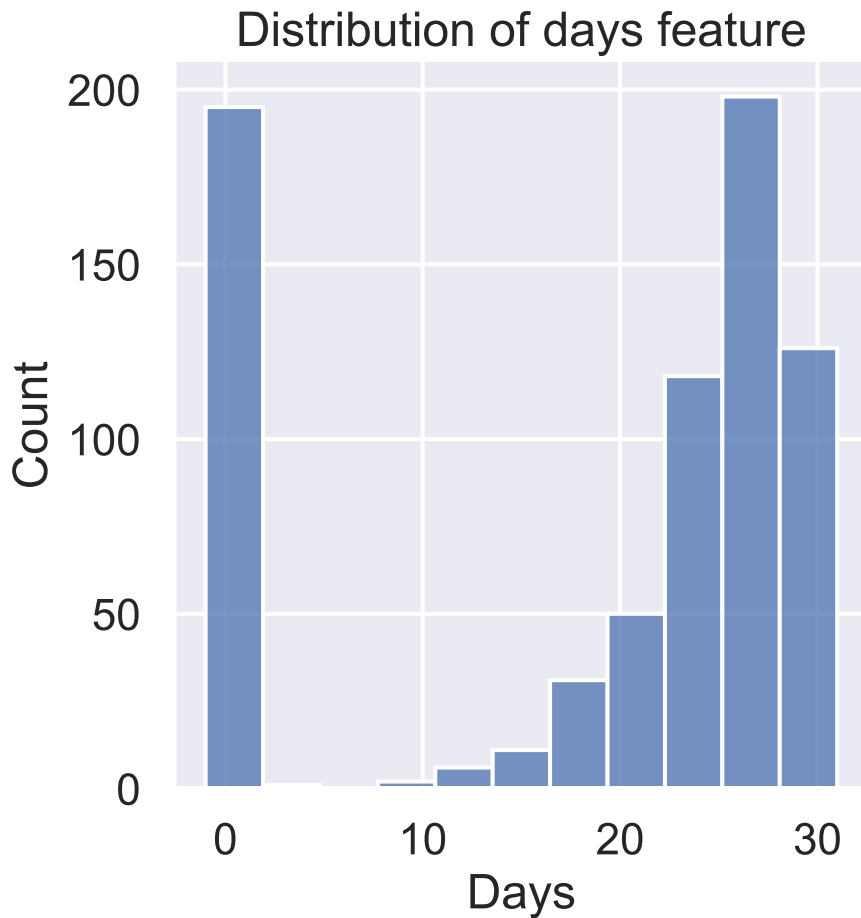
```
co2["Mo"].value_counts().sort_index()
```

```
Mo
1      61
2      61
3      62
4      62
5      62
6      62
7      62
8      62
9      61
10     61
11     61
12     61
Name: count, dtype: int64
```

As expected Jan, Feb, Sep, Oct, Nov, and Dec have 61 occurrences and the rest 62.

Next let's explore **days** **Days** itself, which is the number of days that the measurement equipment worked.

```
sns.displot(co2['Days']);
plt.title("Distribution of days feature"); # suppresses unneeded plotting output
```

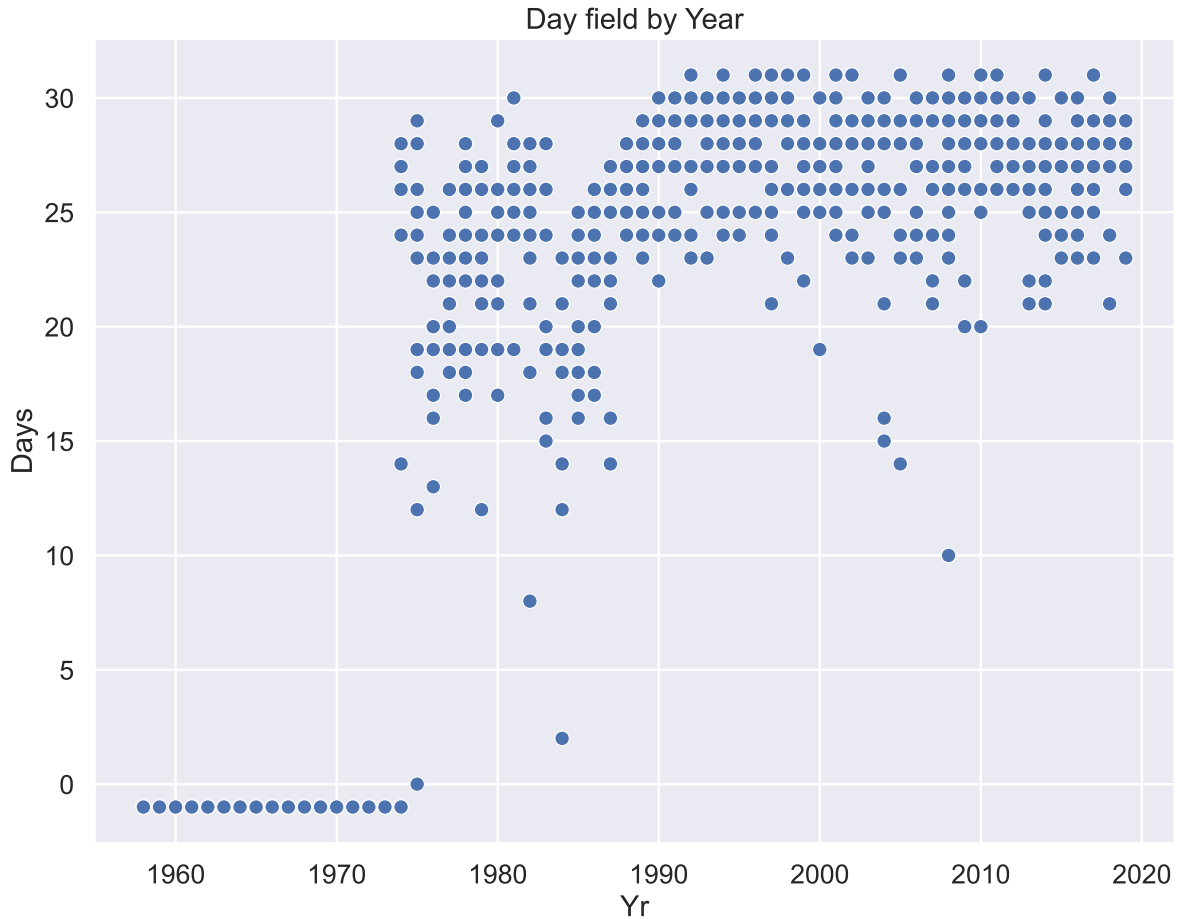


In terms of data quality, a handful of months have averages based on measurements taken on fewer than half the days. In addition, there are nearly 200 missing values—**that’s about 27% of the data!**

Finally, let’s check the last time feature, **year Yr**.

Let’s check to see if there is any connection between missing-ness and the year of the recording.

```
sns.scatterplot(x="Yr", y="Days", data=co2);
plt.title("Day field by Year"); # the ; suppresses output
```



#### Observations:

- All of the missing data are in the early years of operation.
- It appears there may have been problems with equipment in the mid to late 80s.

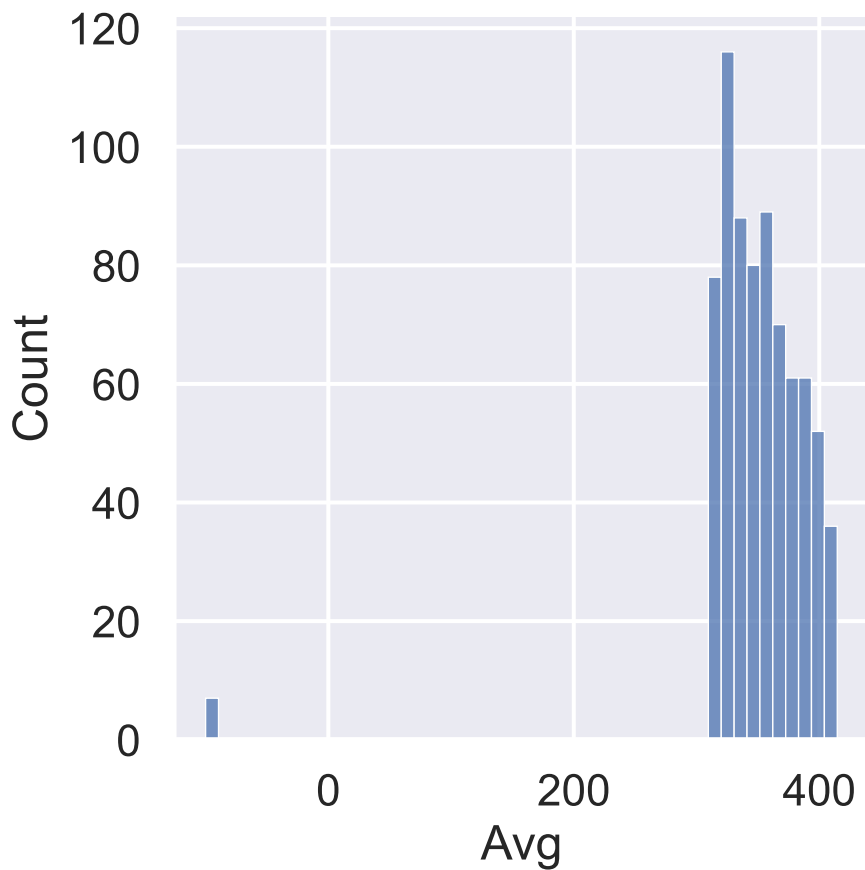
#### Potential Next Steps:

- Confirm these explanations through documentation about the historical readings.
- Maybe drop the earliest recordings? However, we would want to delay such action until after we have examined the time trends and assess whether there are any potential problems.

### 5.5.6 Understanding Missing Value 2: Avg

Next, let's return to the -99.99 values in Avg to analyze the overall quality of the CO2 measurements. We'll plot a histogram of the average CO2 measurements

```
# Histograms of average CO2 measurements
sns.displot(co2['Avg']);
```



The non-missing values are in the 300-400 range (a regular range of CO2 levels).

We also see that there are only a few missing Avg values (<1% of values). Let's examine all of them:

```
co2[co2["Avg"] < 0]
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
3	1958	6	1958.46	-99.99	317.10	314.85	-1
7	1958	10	1958.79	-99.99	312.66	315.61	-1
71	1964	2	1964.12	-99.99	320.07	319.61	-1
72	1964	3	1964.21	-99.99	320.73	319.55	-1



	Yr	Mo	DecDate	Avg	Int	Trend	Days
73	1964	4	1964.29	-99.99	321.77	319.48	-1
213	1975	12	1975.96	-99.99	330.59	331.60	0
313	1984	4	1984.29	-99.99	346.84	344.27	2

There doesn't seem to be a pattern to these values, other than that most records also were missing `Days` data.

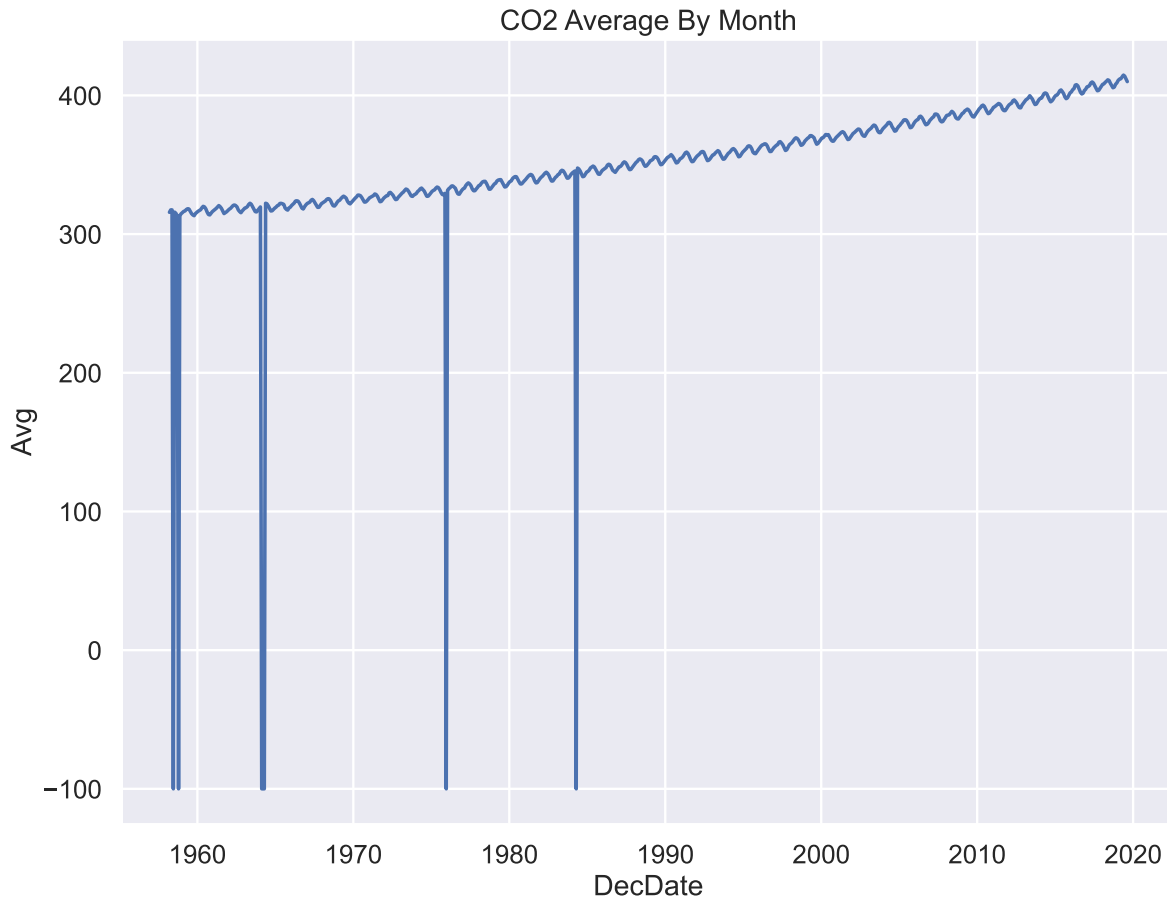
### 5.5.7 Drop, NaN, or Impute Missing Avg Data?

How should we address the invalid `Avg` data?

1. Drop records
2. Set to NaN
3. Impute using some strategy

Remember we want to fix the following plot:

```
sns.lineplot(x='DecDate', y='Avg', data=co2)
plt.title("CO2 Average By Month");
```



Since we are plotting **Avg** vs **DecDate**, we should just focus on dealing with missing values for **Avg**.

Let's consider a few options: 1. Drop those records 2. Replace -99.99 with NaN 3. Substitute it with a likely value for the average CO2?

What do you think are the pros and cons of each possible action?

Let's examine each of these three options.

```
# 1. Drop missing values
co2_drop = co2[co2['Avg'] > 0]
co2_drop.head()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
0	1958	3	1958.21	315.71	315.71	314.62	-1
1	1958	4	1958.29	317.45	317.45	315.29	-1

	Yr	Mo	DecDate	Avg	Int	Trend	Days
2	1958	5	1958.38	317.50	317.50	314.71	-1
4	1958	7	1958.54	315.86	315.86	314.98	-1
5	1958	8	1958.62	314.93	314.93	315.94	-1

```
# 2. Replace NaN with -99.99
co2_NA = co2.replace(-99.99, np.nan)
co2_NA.head()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
0	1958	3	1958.21	315.71	315.71	314.62	-1
1	1958	4	1958.29	317.45	317.45	315.29	-1
2	1958	5	1958.38	317.50	317.50	314.71	-1
3	1958	6	1958.46	NaN	317.10	314.85	-1
4	1958	7	1958.54	315.86	315.86	314.98	-1

We'll also use a third version of the data.

First, we note that the dataset already comes with a **substitute value** for the -99.99.

From the file description:

The **interpolated** column includes average values from the preceding column (**average**) and **interpolated values** where data are missing. Interpolated values are computed in two steps...

The **Int** feature has values that exactly match those in **Avg**, except when **Avg** is -99.99, and then a **reasonable** estimate is used instead.

So, the third version of our data will use the **Int** feature instead of **Avg**.

```
# 3. Use interpolated column which estimates missing Avg values
co2_impute = co2.copy()
co2_impute['Avg'] = co2['Int']
co2_impute.head()
```

	Yr	Mo	DecDate	Avg	Int	Trend	Days
0	1958	3	1958.21	315.71	315.71	314.62	-1
1	1958	4	1958.29	317.45	317.45	315.29	-1
2	1958	5	1958.38	317.50	317.50	314.71	-1

	Yr	Mo	DecDate	Avg	Int	Trend	Days
3	1958	6	1958.46	317.10	317.10	314.85	-1
4	1958	7	1958.54	315.86	315.86	314.98	-1

What's a **reasonable** estimate?

To answer this question, let's zoom in on a short time period, say the measurements in 1958 (where we know we have two missing values).

```
# results of plotting data in 1958

def line_and_points(data, ax, title):
    # assumes single year, hence Mo
    ax.plot('Mo', 'Avg', data=data)
    ax.scatter('Mo', 'Avg', data=data)
    ax.set_xlim(2, 13)
    ax.set_title(title)
    ax.set_xticks(np.arange(3, 13))

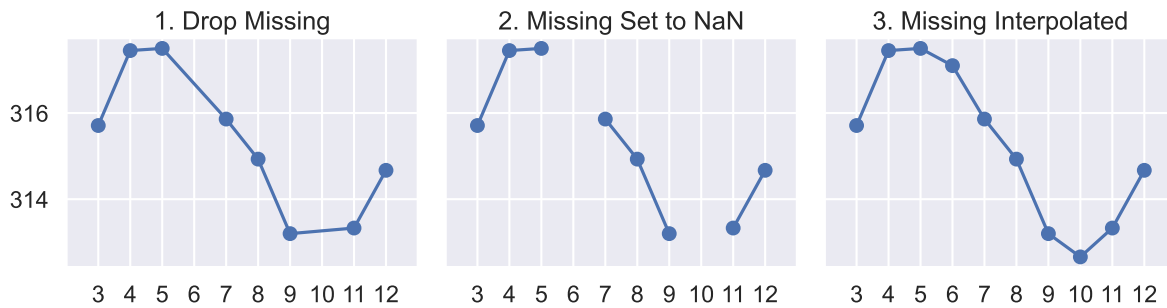
def data_year(data, year):
    return data[data["Yr"] == 1958]

# uses matplotlib subplots
# you may see more next week; focus on output for now
fig, axes = plt.subplots(ncols = 3, figsize=(12, 4), sharey=True)

year = 1958
line_and_points(data_year(co2_drop, year), axes[0], title="1. Drop Missing")
line_and_points(data_year(co2_NA, year), axes[1], title="2. Missing Set to NaN")
line_and_points(data_year(co2_impute, year), axes[2], title="3. Missing Interpolated")

fig.suptitle(f"Monthly Averages for {year}")
plt.tight_layout()
```

## Monthly Averages for 1958



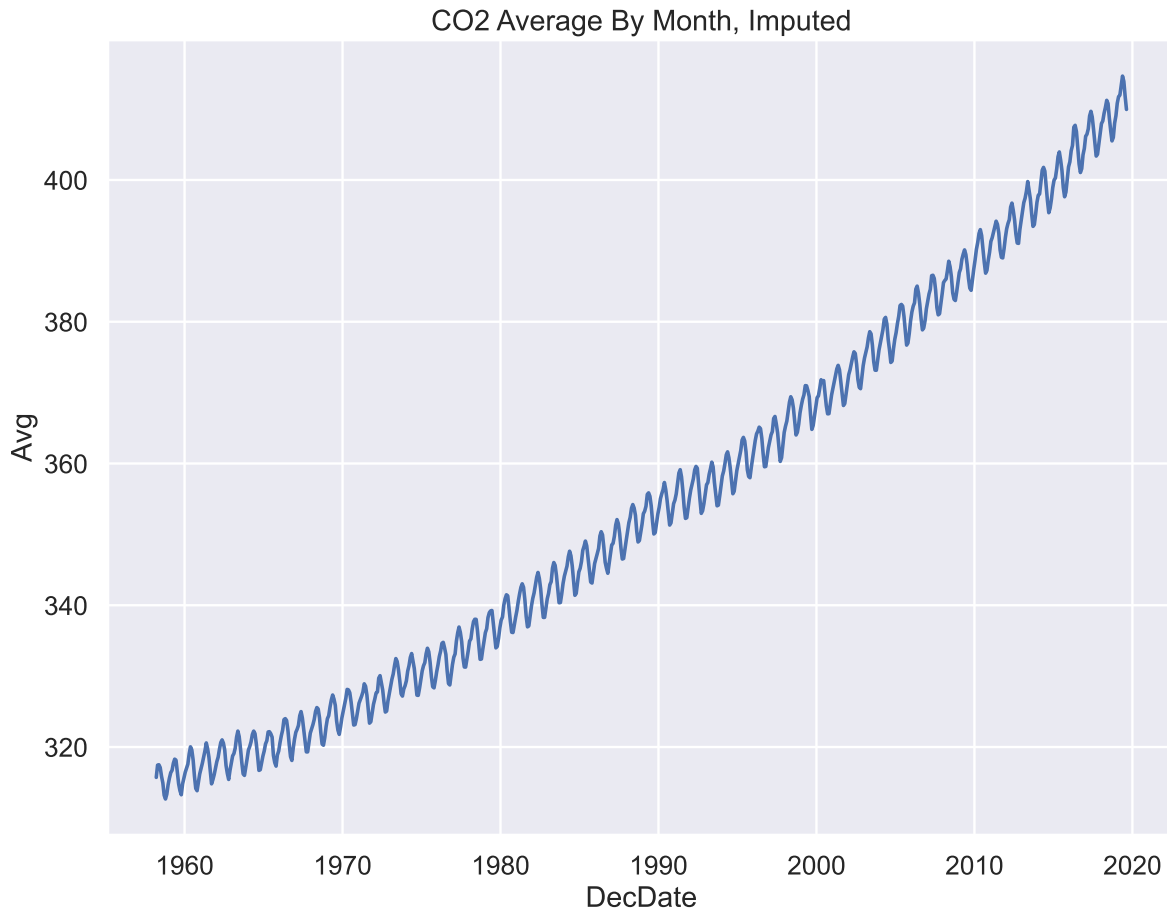
In the big picture since there are only 7 Avg values missing (<1% of 738 months), any of these approaches would work.

However there is some appeal to **option C, Imputing**:

- Shows seasonal trends for CO2
- We are plotting all months in our data as a line plot

Let's replot our original figure with option 3:

```
sns.lineplot(x='DecDate', y='Avg', data=co2_impute)
plt.title("CO2 Average By Month, Imputed");
```



Looks pretty close to what we see on the NOAA [website](#)!

### 5.5.8 Presenting the Data: A Discussion on Data Granularity

From the description:

- Monthly measurements are averages of average day measurements.
- The NOAA GML website has datasets for daily/hourly measurements too.

The data you present depends on your research question.

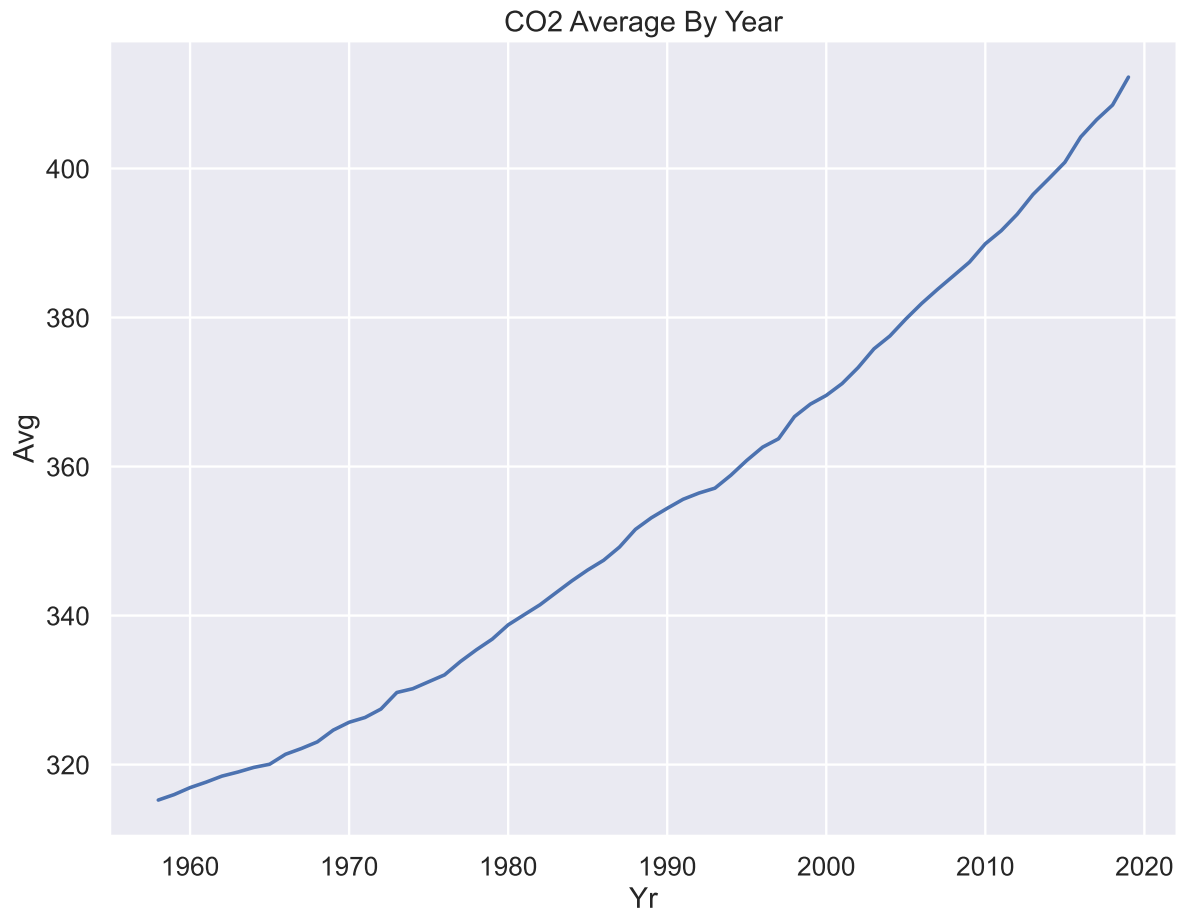
**How do CO2 levels vary by season?**

- You might want to keep average monthly data.

**Are CO2 levels rising over the past 50+ years, consistent with global warming predictions?**

- You might be happier with a **coarser granularity** of average year data!

```
co2_year = co2_impute.groupby('Yr').mean()
sns.lineplot(x='Yr', y='Avg', data=co2_year)
plt.title("CO2 Average By Year");
```



Indeed, we see a rise by nearly 100 ppm of CO2 since Mauna Loa began recording in 1958.

## 5.6 Summary

We went over a lot of content this lecture; let's summarize the most important points:

### 5.6.1 Dealing with Missing Values

There are a few options we can take to deal with missing data:

- Drop missing records
- Keep NaN missing values
- Impute using an interpolated column

### 5.6.2 EDA and Data Wrangling

There are several ways to approach EDA and Data Wrangling:

- Examine the **data and metadata**: what is the date, size, organization, and structure of the data?
- Examine each **field/attribute/dimension** individually.
- Examine pairs of related dimensions (e.g. breaking down grades by major).
- Along the way, we can:
  - **Visualize** or summarize the data.
  - **Validate assumptions** about data and its collection process. Pay particular attention to when the data was collected.
  - Identify and **address anomalies**.
  - Apply data transformations and corrections (we'll cover this in the upcoming lecture).
  - **Record everything you do!** Developing in Jupyter Notebook promotes *reproducibility* of your own work!



## 6 Regular Expressions

### Learning Outcomes

- Understand Python string manipulation, **pandas Series** methods
- Parse and create regex, with a reference table
- Use vocabulary (closure, metacharacters, groups, etc.) to describe regex metacharacters

### 6.1 Why Work with Text?

Last lecture, we learned of the difference between quantitative and qualitative variable types. The latter includes string data — the primary focus of lecture 6. In this note, we'll discuss the necessary tools to manipulate text: Python string manipulation and regular expressions.

There are two main reasons for working with text.

1. Canonicalization: Convert data that has multiple formats into a standard form.
  - By manipulating text, we can join tables with mismatched string labels.
2. Extract information into a new feature.
  - For example, we can extract date and time features from text.

### 6.2 Python String Methods

First, we'll introduce a few methods useful for string manipulation. The following table includes a number of string operations supported by Python and **pandas**. The Python functions operate on a single string, while their equivalent in **pandas** are **vectorized** — they operate on a **Series** of string data.

Operation	Python	Pandas (Series)
Transformation	<ul style="list-style-type: none"><li>• <code>s.lower()</code></li><li>• <code>s.upper()</code></li></ul>	<ul style="list-style-type: none"><li>• <code>ser.str.lower()</code></li><li>• <code>ser.str.upper()</code></li></ul>

Operation	Python	Pandas (Series)
Replacement + Deletion	• <code>s.replace(_)</code>	• <code>ser.str.replace(_)</code>
Split	• <code>s.split(_)</code>	• <code>ser.str.split(_)</code>
Substring	• <code>s[1:4]</code>	• <code>ser.str[1:4]</code>
Membership	• <code>'_' in s</code>	• <code>ser.str.contains(_)</code>
Length	• <code>len(s)</code>	• <code>ser.str.len()</code>

We'll discuss the differences between Python string functions and `pandas` Series methods in the following section on canonicalization.

### 6.2.1 Canonicalization

Assume we want to merge the given tables.

```
import pandas as pd

with open('data/county_and_state.csv') as f:
    county_and_state = pd.read_csv(f)

with open('data/county_and_population.csv') as f:
    county_and_pop = pd.read_csv(f)
```

```
display(county_and_state), display(county_and_pop);
```

	County	State
0	De Witt County	IL
1	Lac qui Parle County	MN
2	Lewis and Clark County	MT
3	St John the Baptist Parish	LS

	County	Population
0	DeWitt	16798
1	Lac Qui Parle	8067
2	Lewis & Clark	55716
3	St. John the Baptist	43044

Can we convert these columns into one standard, canonical form to merge the two tables?

### 6.2.1.1 Canonicalization with Python String Manipulation

The following function uses Python string manipulation to convert a single county name into canonical form. It does so by eliminating whitespace, punctuation, and unnecessary text.

```
def canonicalize_county(county_name):
    return (
        county_name
        .lower()
        .replace(' ', '')
        .replace('&', 'and')
        .replace('.', '')
        .replace('county', '')
        .replace('parish', '')
    )

canonicalize_county("St. John the Baptist")
```

'stjohnthebaptist'

### 6.2.1.2 Canonicalization with Pandas Series Methods

Alternatively, we can use `pandas Series` methods to create this standardized column. To do so, we must call the `.str` attribute of our `Series` object prior to calling any methods, like `.lower` and `.replace`. Notice how these method names match their equivalent built-in Python string functions.

Chaining multiple `Series` methods in this manner eliminates the need to use the `map` function (as this code is vectorized).

```
def canonicalize_county_series(county_series):
    return (
        county_series
        .str.lower()
        .str.replace(' ', '')
        .str.replace('&', 'and')
        .str.replace('.', '')
        .str.replace('county', '')
        .str.replace('parish', '')
    )

county_and_pop['clean_county_pandas'] = canonicalize_county_series(county_and_pop['County'])
```

```
county_and_state['clean_county_pandas'] = canonicalize_county_series(county_and_state['County'],
display(county_and_pop), display(county_and_state));
```

	County	Population	clean_county_pandas
0	DeWitt	16798	dewitt
1	Lac Qui Parle	8067	lacquiparle
2	Lewis & Clark	55716	lewisandclark
3	St. John the Baptist	43044	stjohnthebaptist

	County	State	clean_county_pandas
0	De Witt County	IL	dewitt
1	Lac qui Parle County	MN	lacquiparle
2	Lewis and Clark County	MT	lewisandclark
3	St John the Baptist Parish	LS	stjohnthebaptist

## 6.2.2 Extraction

Extraction explores the idea of obtaining useful information from text data. This will be particularly important in model building, which we'll study in a few weeks.

Say we want to read some data from a `.txt` file.

```
with open('data/log.txt', 'r') as f:
    log_lines = f.readlines()
```

```
log_lines
```

```
['169.237.46.168 - - [26/Jan/2014:10:47:58 -0800] "GET /stat141/Winter04/ HTTP/1.1" 200 2585
'193.205.203.3 - - [2/Feb/2005:17:23:6 -0800] "GET /stat141/Notes/dim.html HTTP/1.0" 404 30
'169.237.46.240 - - [3/Feb/2006:10:18:37 -0800] "GET /stat141/homework/Solutions/hw1Sol.pdf
```

Suppose we want to extract the day, month, year, hour, minutes, seconds, and time zone. Unfortunately, these items are not in a fixed position from the beginning of the string, so slicing by some fixed offset won't work.

Instead, we can use some clever thinking. Notice how the relevant information is contained within a set of brackets, further separated by `/` and `:`. We can hone in on this region of text, and split the data on these characters. Python's built-in `.split` function makes this easy.

```

first = log_lines[0] # Only considering the first row of data

pertinent = first.split("[")[1].split(' ')[0]
day, month, rest = pertinent.split('/')
year, hour, minute, rest = rest.split(':')
seconds, time_zone = rest.split(' ')
day, month, year, hour, minute, seconds, time_zone

```

```
('26', 'Jan', '2014', '10', '47', '58', '-0800')
```

There are two problems with this code:

1. Python's built-in functions limit us to extract data one record at a time,
2. The code is quite verbose.
  - This is a larger issue that is trickier to solve

In the next section, we'll introduce regular expressions - a tool that solves problem 2.

## 6.3 RegEx Basics

A **regular expression** (“**RegEx**”) is a sequence of characters that specifies a search pattern. They are written to extract specific information from text. Regular expressions are essentially part of a smaller programming language embedded in Python, made available through the `re` module. As such, they have a stand-alone syntax and methods for various capabilities.

Regular expressions are useful in many applications beyond data science. For example, Social Security Numbers (SSNs) are often validated with regular expressions.

```

r"[0-9]{3}-[0-9]{2}-[0-9]{4}" # Regular Expression Syntax

# 3 of any digit, then a dash,
# then 2 of any digit, then a dash,
# then 4 of any digit

```

```
'[0-9]{3}-[0-9]{2}-[0-9]{4}'
```

There are a ton of resources to learn and experiment with regular expressions. A few are provided below:

- [Official Regex Guide](#)

- [Data 100 Reference Sheet](#)
- [Regex101.com](#)

– Be sure to check Python under the category on the left.

### 6.3.1 Basics RegEx Syntax

There are four basic operations with regular expressions.

Operation	Order	Syntax Example	Matches	Doesn't Match
Or:	4	AA BAAB	AA BAAB	every other string
Concatenation	3	AABAAB	AABAAB	every other string
Closure: * (zero or more)	2	AB*A	AA ABBBBBBA	AB ABABA
Group: () (parenthesis)	1	A(A B)AAB (AB)*A	AAAAB ABAAB A ABABABABA	every other string AA ABBA

Notice how these metacharacter operations are ordered. Rather than being literal characters, these **metacharacters** manipulate adjacent characters. () takes precedence, followed by \*, and finally |. This allows us to differentiate between very different regex commands like **AB\*** and **(AB)\***. The former reads “A then zero or more copies of B”, while the latter specifies “zero or more copies of AB”.

#### 6.3.1.1 Examples

**Question 1:** Give a regular expression that matches **moon**, **mooon**, etc. Your expression should match any even number of **o**s except zero (i.e. don't match **mn**).

Answer1

**moo(oo)\*n**

- Hardcoding **oo** before the capture group ensures that **mn** is not matched.
- A capture group of **(oo)\*** ensures the number of **o**'s is even.

**Question 2:** Using only basic operations, formulate a regex that matches `muun`, `muuuun`, `moon`, `mooon`, etc. Your expression should match any even number of `us` or `os` except zero (i.e. don't match `mn`).

Answer2

`m(uu(uu)*|oo(oo)*)n`

- The leading `m` and trailing `n` ensures that only strings beginning with `m` and ending with `n` are matched.
- Notice how the outer capture group surrounds the `|`.
  - Consider the regex `m(uu(uu)*)|(oo(oo)*)n`. This incorrectly matches `muu` and `ooon`.
    - \* Each OR clause is everything to the left and right of `|`. The incorrect solution matches only half of the string, and ignores either the beginning `m` or trailing `n`.
    - \* A set of parenthesis must surround `|`. That way, each OR clause is everything to the left and right of `|` **within** the group. This ensures both the beginning `m` and trailing `n` are matched.

## 6.4 RegEx Expanded

Provided below are more complex regular expression functions.

Operation	Syntax Example	Matches	Doesn't Match
Any Character: <code>.</code> (except newline)	<code>.U.U.U.</code>	CUMULUS JUGULUM	SUCCUBUS TUMUL- TUOUS
Character Class: <code>[]</code> (match one character in <code>[]</code> )	<code>[A-Za-z][a-z]*</code>	word Capitalized	camelCase 4illegal
Repeated "a" Times: <code>{a}</code>	<code>j[aeiou]{3}hn</code>	jaoehn jooohn	jhn jaeiouhn
Repeated "from a to b" Times: <code>{a, b}</code>	<code>j[ou]{1,2}hn</code>	john juohn	jhn jooohn
At Least One: <code>+</code>	<code>jo+hn</code>	john joooooooohn	jhn jjohn
Zero or One: <code>?</code>	<code>joh?n</code>	jon john	any other string

A character class matches a single character in its class. These characters can be hardcoded — in the case of `[aeiou]` — or shorthand can be specified to mean a range of characters. Examples include:

1. `[A-Z]`: Any capitalized letter
2. `[a-z]`: Any lowercase letter
3. `[0-9]`: Any single digit
4. `[A-Za-z]`: Any capitalized or lowercase letter
5. `[A-Za-z0-9]`: Any capitalized or lowercase letter or single digit

### 6.4.0.1 Examples

Let's analyze a few examples of complex regular expressions.

Matches	Does Not Match
1. <code>.*SPB.*</code> RASPBERRY SPBOO	SUBSPACE SUBSPECIES
2. <code>[0-9]{3}-[0-9]{2}-[0-9]{4}</code> 231-41-5121 573-57-1821	231415121 57-3571821
3. <code>[a-z]+@([a-z]+\.)+(edu com)</code> horse@pizza.com horse@pizza.food.com	frank_99@yahoo.com hug@cs

### Explanations

1. `.*SPB.*` only matches strings that contain the substring `SPB`.
  - The `.*` metacharacter matches any amount of non-negative characters. Newlines do not count.
2. This regular expression matches 3 of any digit, then a dash, then 2 of any digit, then a dash, then 4 of any digit.
  - You'll recognize this as the familiar Social Security Number regular expression.
3. Matches any email with a `com` or `edu` domain, where all characters of the email are letters.
  - At least one `.` must precede the domain name. Including a backslash `\` before any metacharacter (in this case, the `.`) tells RegEx to match that character exactly.



## 6.5 Convenient RegEx

Here are a few more convenient regular expressions.

Operation	Syntax Example	Matches	Doesn't Match
built in character class	<code>\w+ \d+ \s+</code>	Fawef_03 231123 whitespace	this person 423 people non-whitespace
character class negation: <code>[^]</code> (everything except the given characters)	<code>[^a-z]+.</code>	PEPPERS3982 17211!↑å	porch CLAmS
escape character: <code>\</code> (match the literal next character)	<code>cow\.com</code>	cow.com	cowscom
beginning of line: <code>^</code>	<code>^ark</code>	ark two ark o ark	dark
end of line: <code>\$</code>	<code>ark\$</code>	dark ark o ark	ark two
lazy version of zero or more: <code>*?</code>	<code>5.*?5</code>	5005 55	5005005

### 6.5.1 Greediness

In order to fully understand the last operation in the table, we have to discuss greediness. RegEx is greedy – it will look for the longest possible match in a string. To motivate this with an example, consider the pattern `<div>.*</div>`. In the sentence below, we would hope that the bolded portions would be matched:

“This is a **<div>example</div>** of greediness **<div>in</div>** regular expressions.”

However, in reality, RegEx captures far more of the sentence. The way RegEx processes the text given that pattern is as follows:

1. “Look for the exact string `<div>`”
2. Then, “look for any character 0 or more times”
3. Then, “look for the exact string `</div>`”

The result would be all the characters starting from the leftmost `<div>` and the rightmost `</div>` (inclusive):

“This is a **<div>example</div>** of greediness **<div>in</div>** regular expressions.”

We can fix this by making our pattern non-greedy, `<div>.*?</div>`. You can read up more in the documentation [here](#).

## 6.5.2 Examples

Let's revisit our earlier problem of extracting date/time data from the given `.txt` files. Here is how the data looked.

```
log_lines[0]
```

```
'169.237.46.168 - - [26/Jan/2014:10:47:58 -0800] "GET /stat141/Winter04/ HTTP/1.1" 200 2585'
```

**Question:** Give a regular expression that matches everything contained within and including the brackets - the day, month, year, hour, minutes, seconds, and time zone.

Answer

```
\[.*\]
```

- Notice how matching the literal `[` and `]` is necessary. Therefore, an escape character `\` is required before both `[` and `]` — otherwise these metacharacters will match character classes.
- We need to match a particular format between `[` and `]`. For this example, `.*` will suffice.

**Alternative Solution:** `\[\w+/\w+/\w+:\w+:\w+:\w+\s-\w+\]`

- This solution is much safer.
  - Imagine the data between `[` and `]` was garbage - `.*` will still match that.
  - The alternate solution will only match data that follows the correct format.

## 6.6 Regex in Python and Pandas (RegEx Groups)

### 6.6.1 Canonicalization

#### 6.6.1.1 Canonicalization with RegEx

Earlier in this note, we examined the process of canonicalization using `python` string manipulation and `pandas Series` methods. However, we mentioned this approach had a major flaw: our code was unnecessarily verbose. Equipped with our knowledge of regular expressions, let's fix this.

To do so, we need to understand a few functions in the `re` module. The first of these is the substitute function: `re.sub(pattern, rep1, text)`. It behaves similarly to `python`'s built-in `.replace` function, and returns text with all instances of `pattern` replaced by `rep1`.

The regular expression here removes text surrounded by <> (also known as HTML tags).

In order, the pattern matches ... 1. a single < 2. any character that is not a > : div, td valign..., /td, /div 3. a single >

Any substring in `text` that fulfills all three conditions will be replaced by ''.

```
import re

text = "<div><td valign='top'>Moo</td></div>"
pattern = r"<[^>]+>"
re.sub(pattern, '', text)
```

'Moo'

Notice the `r` preceding the regular expression pattern; this specifies the regular expression is a raw string. Raw strings do not recognize escape sequences (i.e., the Python newline metacharacter `\n`). This makes them useful for regular expressions, which often contain literal `\` characters.

In other words, don't forget to tag your RegEx with an `r`.

### 6.6.1.2 Canonicalization with pandas

We can also use regular expressions with `pandas Series` methods. This gives us the benefit of operating on an entire column of data as opposed to a single value. The code is simple: `ser.str.replace(pattern, repl, regex=True)`.

Consider the following `DataFrame` `html_data` with a single column.

```
data = {"HTML": ["<div><td valign='top'>Moo</td></div>", \
                 "<a href='http://ds100.org'>Link</a>", \
                 "<b>Bold text</b>"]}
html_data = pd.DataFrame(data)
```

`html_data`

	<u>HTML</u>
0	<div><td valign='top'>Moo</td></div>
1	<a href='http://ds100.org'>Link</a>
2	<b>Bold text</b>

```
pattern = r"<[^>]+>"
html_data['HTML'].str.replace(pattern, '', regex=True)
```

```
0      Moo
1      Link
2  Bold text
Name: HTML, dtype: object
```

## 6.6.2 Extraction

### 6.6.2.1 Extraction with RegEx

Just like with canonicalization, the `re` module provides capability to extract relevant text from a string: `re.findall(pattern, text)`. This function returns a list of all matches to `pattern`.

Using the familiar regular expression for Social Security Numbers:

```
text = "My social security number is 123-45-6789 bro, or maybe it's 321-45-6789."
pattern = r"[0-9]{3}-[0-9]{2}-[0-9]{4}"
re.findall(pattern, text)
```

```
['123-45-6789', '321-45-6789']
```

### 6.6.2.2 Extraction with pandas

`pandas` similarly provides extraction functionality on a `Series` of data: `ser.str.findall(pattern)`

Consider the following `DataFrame` `ssn_data`.

```
data = {"SSN": ["987-65-4321", "forty", \
               "123-45-6789 bro or 321-45-6789",
               "999-99-9999"]}
ssn_data = pd.DataFrame(data)
```

```
ssn_data
```

	SSN
0	987-65-4321
1	forty
2	123-45-6789 bro or 321-45-6789
3	999-99-9999

```
ssn_data["SSN"].str.findall(pattern)
```

```
0      [987-65-4321]
1      []
2    [123-45-6789, 321-45-6789]
3      [999-99-9999]
Name: SSN, dtype: object
```

This function returns a list for every row containing the pattern matches in a given string.

As you may expect, there are similar **pandas** equivalents for other **re** functions as well. **Series.str.extract** takes in a pattern and returns a **DataFrame** of each capture group's first match in the string. In contrast, **Series.str.extractall** returns a multi-indexed **DataFrame** of all matches for each capture group. You can see the difference in the outputs below:

```
pattern_cg = r"([0-9]{3})-([0-9]{2})-([0-9]{4})"
ssn_data["SSN"].str.extract(pattern_cg)
```

	0	1	2
0	987	65	4321
1	NaN	NaN	NaN
2	123	45	6789
3	999	99	9999

```
ssn_data["SSN"].str.extractall(pattern_cg)
```

		0	1	2
	match			
0		0	987	65
2		0	123	45
		1	321	45

0	1	2
match		

### 6.6.3 Regular Expression Capture Groups

Earlier we used parentheses ( ) to specify the highest order of operation in regular expressions. However, they have another meaning; parentheses are often used to represent **capture groups**. Capture groups are essentially, a set of smaller regular expressions that match multiple substrings in text data.

Let's take a look at an example.

#### 6.6.3.1 Example 1

```
text = "Observations: 03:04:53 - Horse awakens. \
       03:05:14 - Horse goes back to sleep."
```

Say we want to capture all occurrences of time data (hour, minute, and second) as *separate entities*.

```
pattern_1 = r"(\d\d):(\d\d):(\d\d)"
re.findall(pattern_1, text)
```

```
[('03', '04', '53'), ('03', '05', '14')]
```

Notice how the given pattern has 3 capture groups, each specified by the regular expression (\d\d). We then use `re.findall` to return these capture groups, each as tuples containing 3 matches.

These regular expression capture groups can be different. We can use the (\d{2}) shorthand to extract the same data.

```
pattern_2 = r"(\d\d):(\d\d):(\d{2})"
re.findall(pattern_2, text)
```

```
[('03', '04', '53'), ('03', '05', '14')]
```

### 6.6.3.2 Example 2

With the notion of capture groups, convince yourself how the following regular expression works.

```
first = log_lines[0]
first
```

```
'169.237.46.168 - - [26/Jan/2014:10:47:58 -0800] "GET /stat141/Winter04/ HTTP/1.1" 200 2585'
```

```
pattern = r'\[(\d+)\]/(\w+)\[(\d+):(\d+):(\d+):(\d+) (.+)\]'
day, month, year, hour, minute, second, time_zone = re.findall(pattern, first)[0]
print(day, month, year, hour, minute, second, time_zone)
```

```
26 Jan 2014 10 47 58 -0800
```

## 6.7 Limitations of Regular Expressions

Today, we explored the capabilities of regular expressions in data wrangling with text data. However, there are a few things to be wary of.

Writing regular expressions is like writing a program.

- Need to know the syntax well.
- Can be easier to write than to read.
- Can be difficult to debug.

Regular expressions are terrible at certain types of problems:

- For parsing a hierarchical structure, such as JSON, use the `json.load()` parser, not RegEx!
- Complex features (e.g. valid email address).
- Counting (same number of instances of a and b). (impossible)
- Complex properties (palindromes, balanced parentheses). (impossible)

Ultimately, the goal is not to memorize all regular expressions. Rather, the aim is to:

- Understand what RegEx is capable of.
- Parse and create RegEx, with a reference table
- Use vocabulary (metacharacter, escape character, groups, etc.) to describe regex metacharacters.
- Differentiate between `()`, `[]`, `{}`

- Design your own character classes with `\d`, `\w`, `\s`, `[...-...]`, `^`, etc.
- Use `python` and `pandas` RegEx methods.



# 7 Visualization I

## i Learning Outcomes

- Understand the theories behind effective visualizations and start to generate plots of our own with `matplotlib` and `seaborn`.
- Analyze histograms and identify the skewness, potential outliers, and the mode.
- Use `boxplot` and `violinplot` to compare two distributions.

In our journey of the data science lifecycle, we have begun to explore the vast world of exploratory data analysis. More recently, we learned how to pre-process data using various data manipulation techniques. As we work towards understanding our data, there is one key component missing in our arsenal — the ability to visualize and discern relationships in existing data.

These next two lectures will introduce you to various examples of data visualizations and their underlying theory. In doing so, we'll motivate their importance in real-world examples with the use of plotting libraries.

## 7.1 Visualizations in Data 8 and Data 100 (so far)

You've likely encountered several forms of data visualizations in your studies. You may remember two such examples from Data 8: line plots, scatter plots, and histograms. Each of these served a unique purpose. For example, line plots displayed how numerical quantities changed over time, while histograms were useful in understanding a variable's distribution.

---

Line Chart

---

Scatter Plot

---

---

Histogram

---

## 7.2 Goals of Visualization

Visualizations are useful for a number of reasons. In Data 100, we consider two areas in particular:

1. To broaden your understanding of the data. Summarizing trends visually before in-depth analysis is a key part of exploratory data analysis. Creating these graphs is a lightweight, iterative and flexible process that helps us investigate relationships between variables.
2. To communicate results/conclusions to others. These visualizations are highly editorial, selective, and fine-tuned to achieve a communications goal, so be thoughtful and careful about its clarity, accessibility, and necessary context.

Altogether, these goals emphasize the fact that visualizations aren't a matter of making "pretty" pictures; we need to do a lot of thinking about what stylistic choices communicate ideas most effectively.

This course note will focus on the first half of visualization topics in Data 100. The goal here is to understand how to choose the "right" plot depending on different variable types and, secondly, how to generate these plots using code.

## 7.3 An Overview of Distributions

A distribution describes both the set of values that a single variable can take and the frequency of unique values in a single variable. For example, if we're interested in the distribution of students across Data 100 discussion sections, the set of possible values is a list of discussion sections (10-11am, 11-12pm, etc.), and the frequency that each of those values occur is the number of students enrolled in each section. In other words, we're interested in how a variable is distributed across its possible values. Therefore, distributions must satisfy two properties:

1. The total frequency of all categories must sum to 100%
2. Total count should sum to the total number of datapoints if we're using raw counts.

Not a Valid Distribution	Valid Distribution
This is not a valid distribution since individuals can be associated with more than one category and the bar values demonstrate values in minutes and not probability.	This example satisfies the two properties of distributions, so it is a valid distribution.

## 7.4 Variable Types Should Inform Plot Choice

Different plots are more or less suited for displaying particular types of variables, laid out in the diagram below:

The first step of any visualization is to identify the type(s) of variables we're working with. From here, we can select an appropriate plot type:

## 7.5 Qualitative Variables: Bar Plots

A **bar plot** is one of the most common ways of displaying the **distribution** of a **qualitative** (categorical) variable. The length of a bar plot encodes the frequency of a category; the width encodes no useful information. The color *could* indicate a sub-category, but this is not necessarily the case.

Let's contextualize this in an example. We will use the World Bank dataset (**wb**) in our analysis.

```
import pandas as pd
import numpy as np
import warnings

warnings.filterwarnings("ignore", "use_inf_as_na") # Supresses distracting deprecation warnings

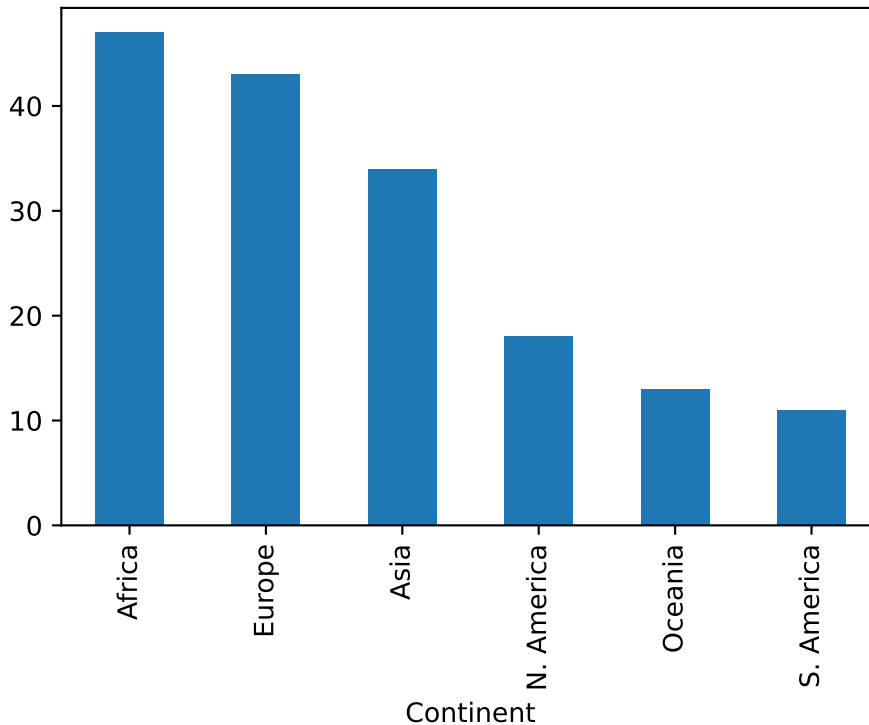
wb = pd.read_csv("data/world_bank.csv", index_col=0)
wb.head()
```

	Continent	Country	Primary completion rate: Male: % of relevant age group: 2015	Primary completion
0	Africa	Algeria	106.0	105.0
1	Africa	Angola	NaN	NaN
2	Africa	Benin	83.0	73.0
3	Africa	Botswana	98.0	101.0
5	Africa	Burundi	58.0	66.0

We can visualize the distribution of the **Continent** column using a bar plot. There are a few ways to do this.

### 7.5.1 Plotting in Pandas

```
wb['Continent'].value_counts().plot(kind='bar');
```



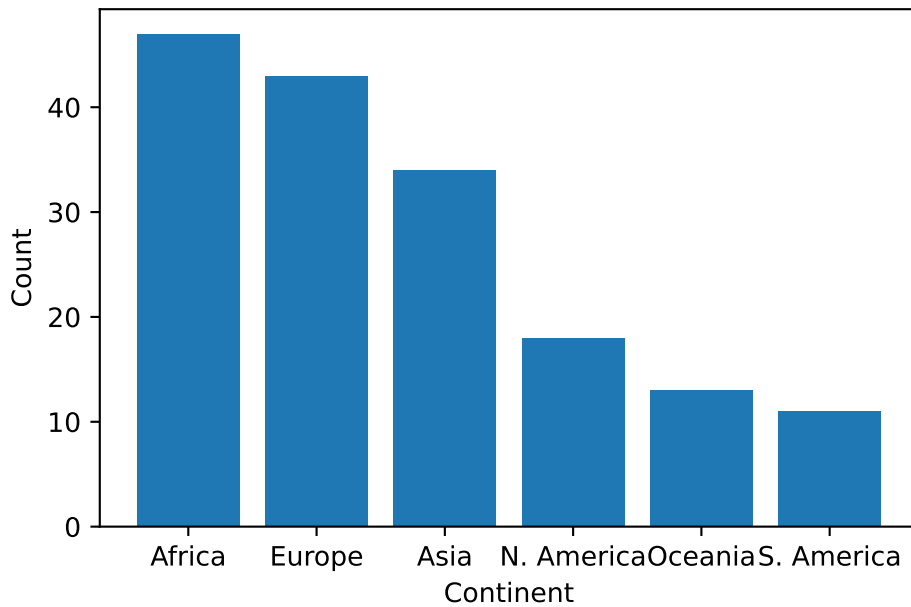
Recall that `.value_counts()` returns a **Series** with the total count of each unique value. We call `.plot(kind='bar')` on this result to visualize these counts as a bar plot.

Plotting methods in **pandas** are the least preferred and not supported in Data 100, as their functionality is limited. Instead, future examples will focus on other libraries built specifically for visualizing data. The most well-known library here is **matplotlib**.

### 7.5.2 Plotting in Matplotlib

```
import matplotlib.pyplot as plt # matplotlib is typically given the alias plt

continent = wb['Continent'].value_counts()
plt.bar(continent.index, continent)
plt.xlabel('Continent')
plt.ylabel('Count');
```

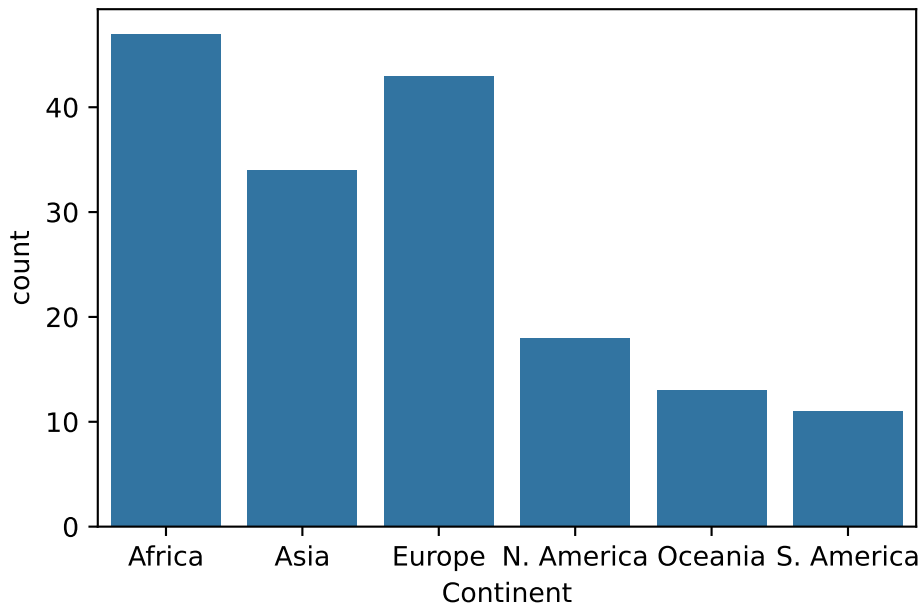


While more code is required to achieve the same result, `matplotlib` is often used over `pandas` for its ability to plot more complex visualizations, some of which are discussed shortly.

However, note how we needed to label the axes with `plt.xlabel` and `plt.ylabel`, as `matplotlib` does not support automatic axis labeling. To get around these inconveniences, we can use a more efficient plotting library: `seaborn`.

### 7.5.3 Plotting in Seaborn

```
import seaborn as sns # seaborn is typically given the alias sns
sns.countplot(data = wb, x = 'Continent');
```



In contrast to `matplotlib`, the general structure of a `seaborn` call involves passing in an entire `DataFrame`, and then specifying what column(s) to plot. `seaborn.countplot` both counts and visualizes the number of unique values in a given column. This column is specified by the `x` argument to `sns.countplot`, while the `DataFrame` is specified by the `data` argument.

`seaborn` is built on `matplotlib`! When using `seaborn`, you're actually using `matplotlib` under the hood, but with an easier-to-use interface for working with `DataFrames` and creating certain types of plots.

For the vast majority of visualizations, `seaborn` is far more concise and aesthetically pleasing than `matplotlib`. However, the color scheme of this particular bar plot is arbitrary - it encodes no additional information about the categories themselves. This is not always true; color may signify meaningful detail in other visualizations. We'll explore this more in-depth during the next lecture.

By now, you'll have noticed that each of these plotting libraries have a very different syntax. As with `pandas`, we'll teach you the important methods in `matplotlib` and `seaborn`, but you'll learn more through documentation.

1. [Matplotlib Documentation](#)
2. [Seaborn Documentation](#)

## 7.6 Distributions of Quantitative Variables

Revisiting our example with the `wb` DataFrame, let's plot the distribution of `Gross national income per capita`.

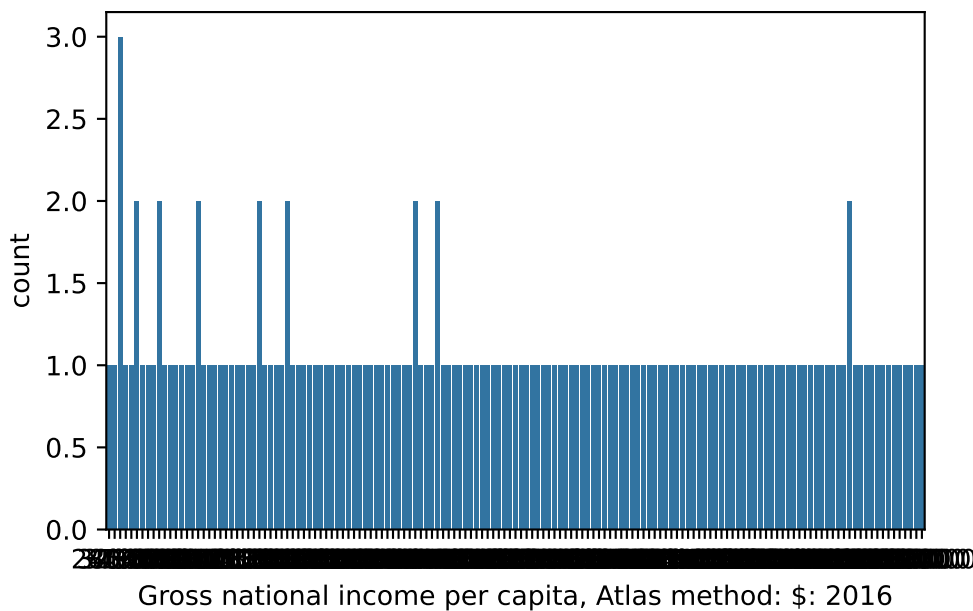
```
wb.head(5)
```

	Continent	Country	Primary completion rate: Male: % of relevant age group: 2015	Primary completion
0	Africa	Algeria	106.0	105.0
1	Africa	Angola	NaN	NaN
2	Africa	Benin	83.0	73.0
3	Africa	Botswana	98.0	101.0
5	Africa	Burundi	58.0	66.0

How should we define our categories for this variable? In the previous example, these were a few unique values of the `Continent` column. If we use similar logic here, our categories are the different numerical values contained in the `Gross national income per capita` column.

Under this assumption, let's plot this distribution using the `seaborn.countplot` function.

```
sns.countplot(data = wb, x = 'Gross national income per capita, Atlas method: $: 2016');
```



What happened? A bar plot (either `plt.bar` or `sns.countplot`) will create a separate bar for each unique value of a variable. With a continuous variable, we may not have a finite number of possible values, which can lead to situations like above where we would need many, many bars to display each unique value.

Specifically, we can say this histogram suffers from **overplotting** as we are unable to interpret the plot and gain any meaningful insight.

Rather than bar plots, to visualize the distribution of a continuous variable, we use one of the following types of plots:

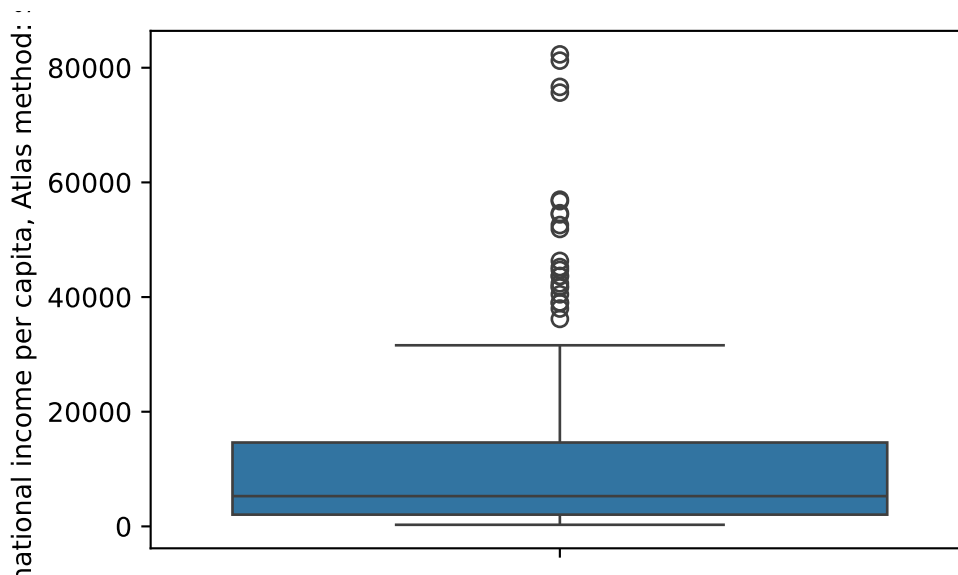
- Histogram
- Box plot
- Violin plot

### 7.6.1 Box Plots and Violin Plots

Box plots and violin plots are two very similar kinds of visualizations. Both display the distribution of a variable using information about **quartiles**.

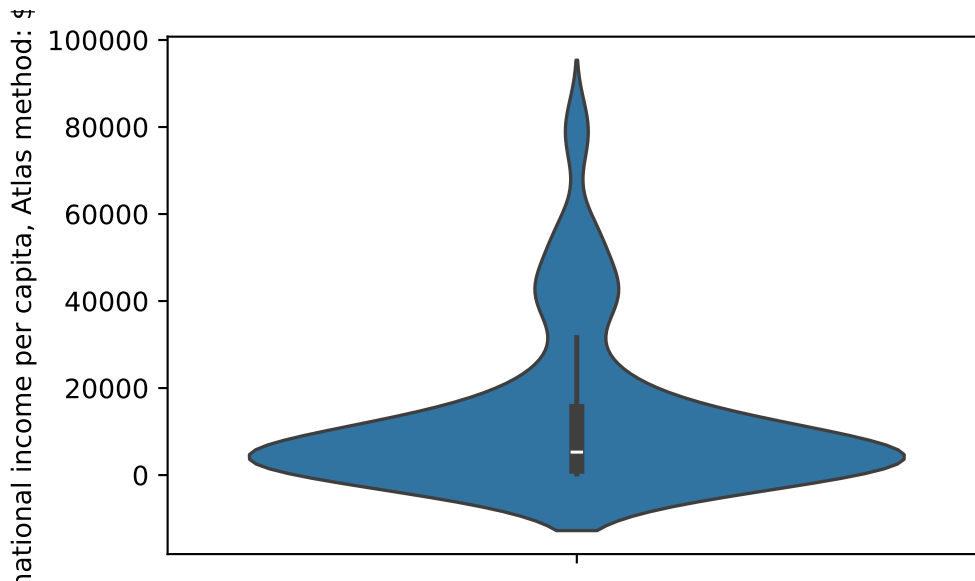
In a box plot, the width of the box at any point does not encode meaning. In a violin plot, the width of the plot indicates the density of the distribution at each possible value.

```
sns.boxplot(data=wb, y='Gross national income per capita, Atlas method: $: 2016');
```





```
sns.violinplot(data=wb, y="Gross national income per capita, Atlas method: $: 2016");
```



A quartile represents a 25% portion of the data. We say that:

- The first quartile (Q1) represents the 25th percentile – 25% of the data is smaller than or equal to the first quartile.
- The second quartile (Q2) represents the 50th percentile, also known as the median – 50% of the data is smaller than or equal to the second quartile.
- The third quartile (Q3) represents the 75th percentile – 75% of the data is smaller than or equal to the third quartile.

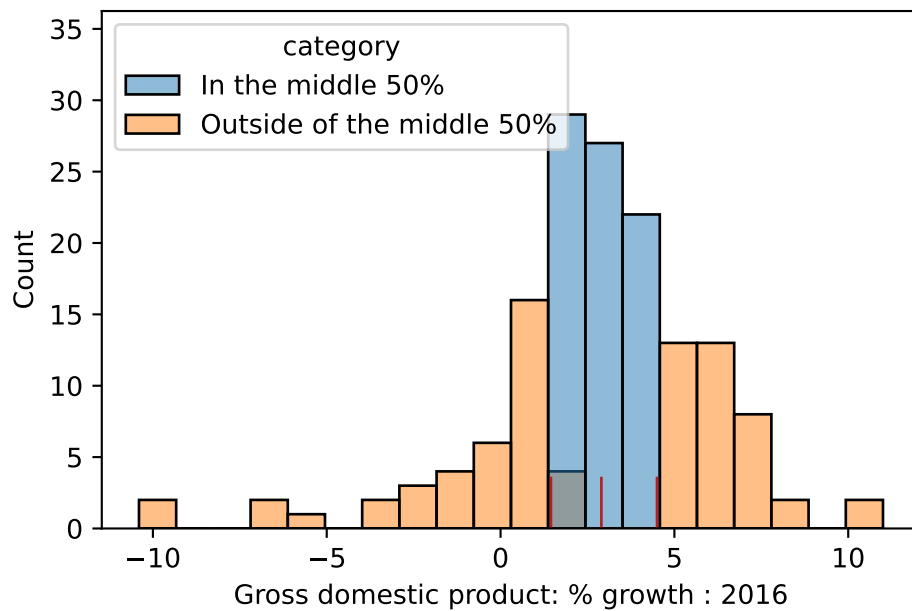
This means that the middle 50% of the data lies between the first and third quartiles. This is demonstrated in the histogram below. The three quartiles are marked with red vertical bars.

```
gdp = wb['Gross domestic product: % growth : 2016']
gdp = gdp[~gdp.isna()]

q1, q2, q3 = np.percentile(gdp, [25, 50, 75])

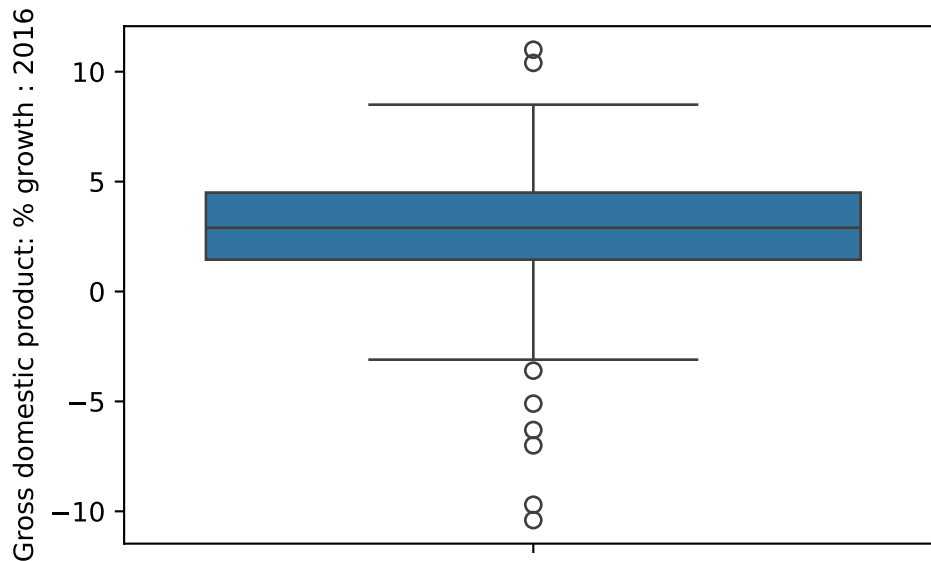
wb_quartiles = wb.copy()
wb_quartiles['category'] = None
wb_quartiles.loc[(wb_quartiles['Gross domestic product: % growth : 2016'] < q1) | (wb_quartiles['Gross domestic product: % growth : 2016'] > q3)] = 'Outside Quartiles'
wb_quartiles.loc[(wb_quartiles['Gross domestic product: % growth : 2016'] >= q1) & (wb_quartiles['Gross domestic product: % growth : 2016'] <= q3)] = 'Inside Quartiles'
```

```
sns.histplot(wb_quartiles, x="Gross domestic product: % growth : 2016", hue="category")
sns.rugplot([q1, q2, q3], c="firebrick", lw=6, height=0.1);
```



In a box plot, the lower extent of the box lies at Q1, while the upper extent of the box lies at Q3. The horizontal line in the middle of the box corresponds to Q2 (equivalently, the median).

```
sns.boxplot(data=wb, y='Gross domestic product: % growth : 2016');
```

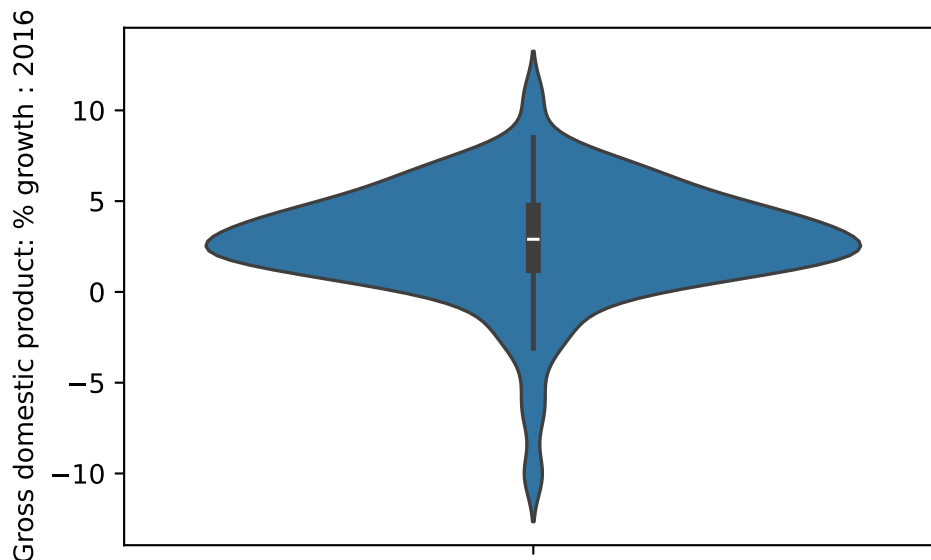


The **whiskers** of a box-plot are the two points that lie at the  $[1^{st} \text{ Quartile} - (1.5 \times \text{IQR})]$ , and the  $[3^{rd} \text{ Quartile} + (1.5 \times \text{IQR})]$ . They are the lower and upper ranges of “normal” data (the points excluding outliers).

The different forms of information contained in a box plot can be summarised as follows:

A violin plot displays quartile information, albeit a bit more subtly through smoothed density curves. Look closely at the center vertical bar of the violin plot below; the three quartiles and “whiskers” are still present!

```
sns.violinplot(data=wb, y='Gross domestic product: % growth : 2016');
```

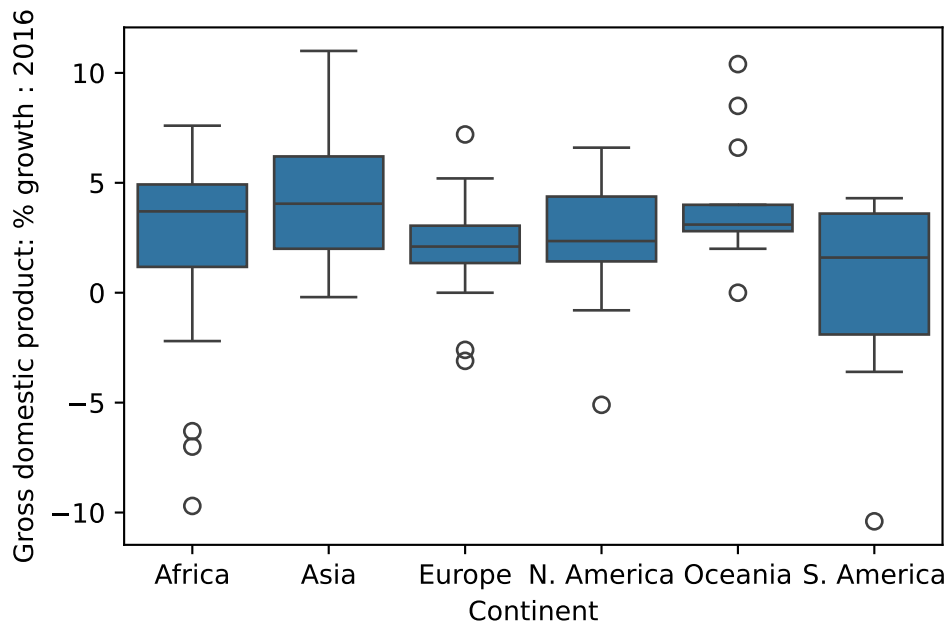


## 7.6.2 Side-by-Side Box and Violin Plots

Plotting side-by-side box or violin plots allows us to compare distributions across different categories. In other words, they enable us to plot both a qualitative variable and a quantitative continuous variable in one visualization.

With `seaborn`, we can easily create side-by-side plots by specifying both an x and y column.

```
sns.boxplot(data=wb, x="Continent", y='Gross domestic product: % growth : 2016');
```



## 7.6.3 Histograms

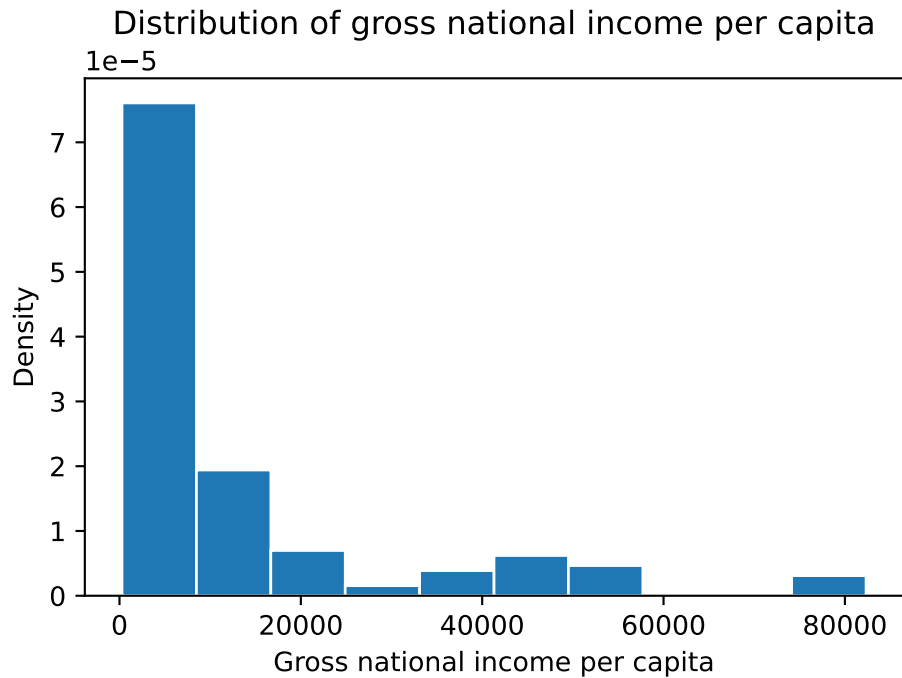
You are likely familiar with histograms from Data 8. A histogram collects continuous data into bins, then plots this binned data. Each bin reflects the density of datapoints with values that lie between the left and right ends of the bin; in other words, the **area** of each bin is proportional to the **percentage** of datapoints it contains.

### 7.6.3.1 Plotting Histograms

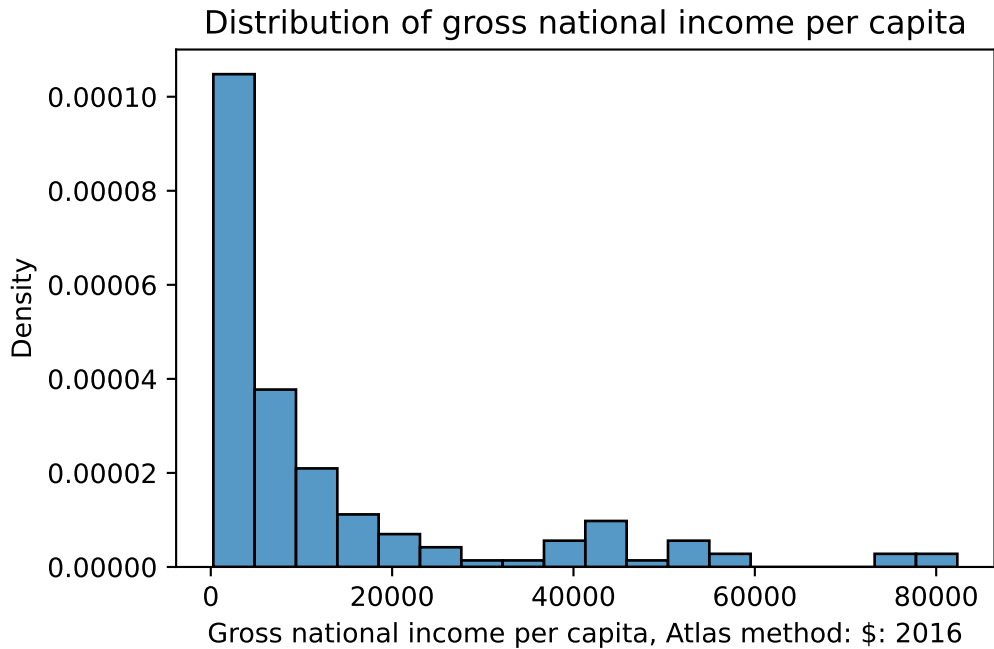
Below, we plot a histogram using `matplotlib` and `seaborn`. Which graph do you prefer?

```
# The `edgecolor` argument controls the color of the bin edges
gni = wb["Gross national income per capita, Atlas method: $: 2016"]
plt.hist(gni, density=True, edgecolor="white")

# Add labels
plt.xlabel("Gross national income per capita")
plt.ylabel("Density")
plt.title("Distribution of gross national income per capita");
```



```
sns.histplot(data=wb, x="Gross national income per capita, Atlas method: $: 2016", stat="density")
plt.title("Distribution of gross national income per capita");
```



### 7.6.3.2 Overlaid Histograms

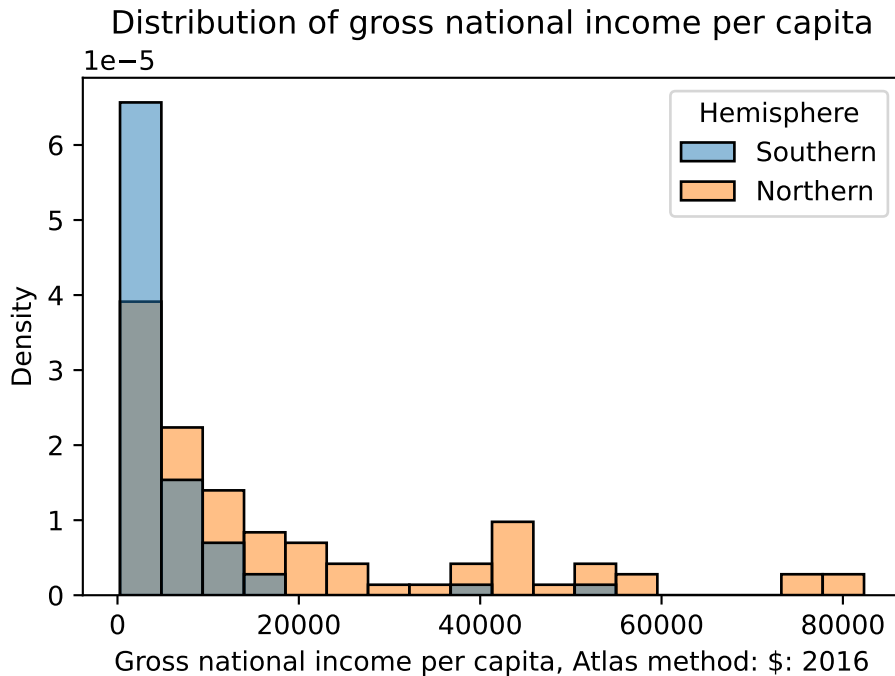
We can overlay histograms (or density curves) to compare distributions across qualitative categories.

The `hue` parameter of `sns.histplot` specifies the column that should be used to determine the color of each category. `hue` can be used in many `seaborn` plotting functions.

Notice that the resulting plot includes a legend describing which color corresponds to each hemisphere – a legend should always be included if color is used to encode information in a visualization!

```
# Create a new variable to store the hemisphere in which each country is located
north = ["Asia", "Europe", "N. America"]
south = ["Africa", "Oceania", "S. America"]
wb.loc[wb["Continent"].isin(north), "Hemisphere"] = "Northern"
wb.loc[wb["Continent"].isin(south), "Hemisphere"] = "Southern"
```

```
sns.histplot(data=wb, x="Gross national income per capita, Atlas method: $: 2016", hue="Hemisphere",
plt.title("Distribution of gross national income per capita");
```



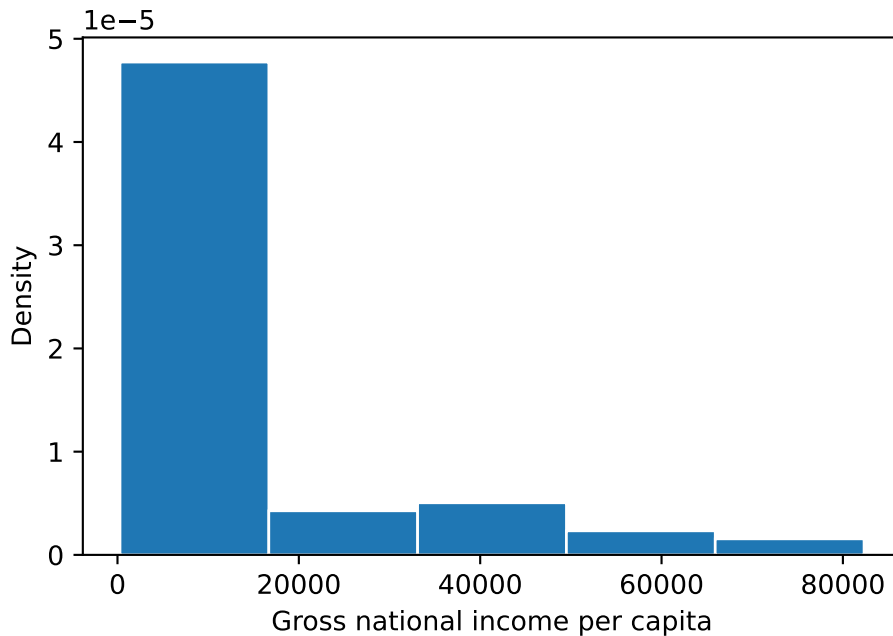
Again, each bin of a histogram is scaled such that its **area** is proportional to the **percentage** of all datapoints that it contains.

```
densities, bins, _ = plt.hist(gni, density=True, edgecolor="white", bins=5)
plt.xlabel("Gross national income per capita")
plt.ylabel("Density")

print(f"First bin has width {bins[1]-bins[0]} and height {densities[0]}")
print(f"This corresponds to {bins[1]-bins[0]} * {densities[0]} = {(bins[1]-bins[0])*densities[0]} of the data")
```

First bin has width 16410.0 and height 4.7741589911386953e-05

This corresponds to 16410.0 \* 4.7741589911386953e-05 = 78.343949044586% of the data



### 7.6.3.3 Evaluating Histograms

Histograms allow us to assess a distribution by their shape. There are a few properties of histograms we can analyze:

1. Skewness and Tails
  - Skewed left vs skewed right
  - Left tail vs right tail
2. Outliers
  - Using percentiles
3. Modes
  - Most commonly occurring data

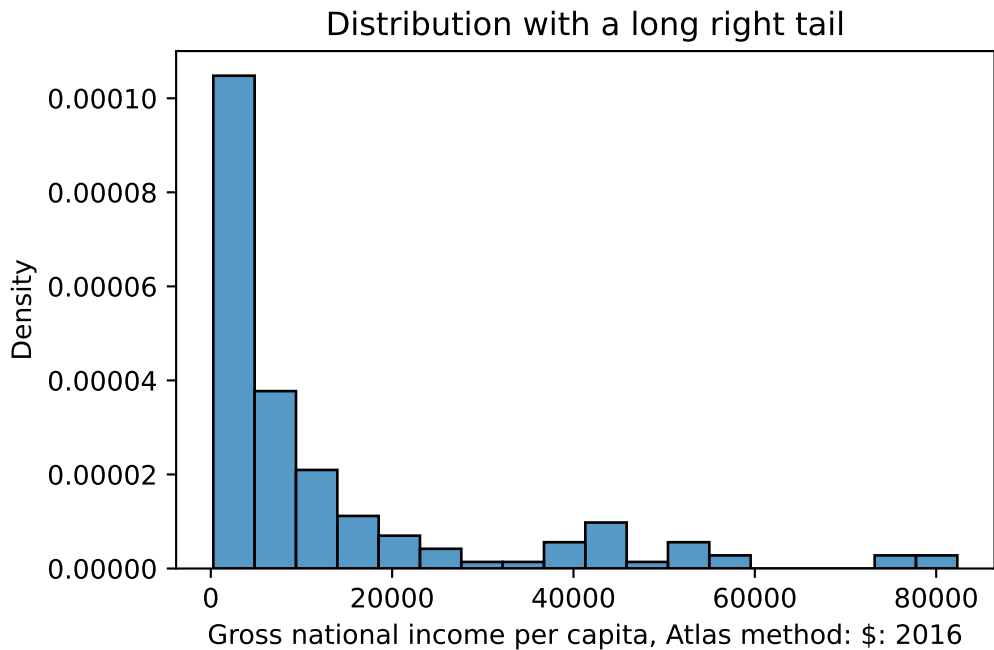
#### 7.6.3.3.1 Skewness and Tails

The skew of a histogram describes the direction in which its “tail” extends. - A distribution with a long right tail is **skewed right** (such as **Gross national income per capita**). In a right-skewed distribution, the few large outliers “pull” the mean to the **right** of the median.



```
sns.histplot(data = wb, x = 'Gross national income per capita, Atlas method: $: 2016', stat = 'density')
plt.title('Distribution with a long right tail')
```

Text(0.5, 1.0, 'Distribution with a long right tail')

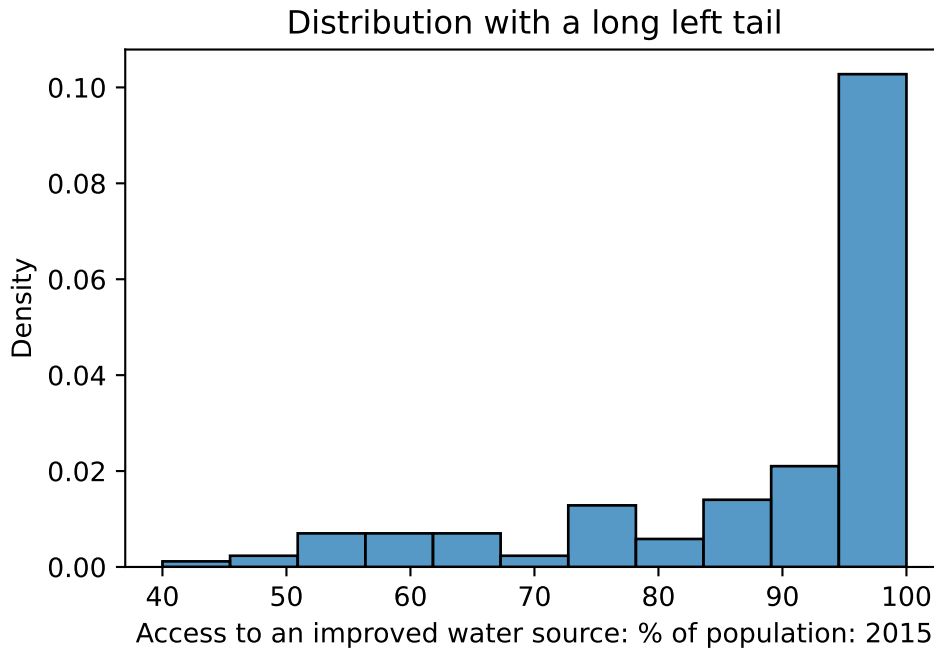


- A distribution with a long left tail is **skewed left** (such as Access to an improved water source). In a left-skewed distribution, the few small outliers “pull” the mean to the **left** of the median.

In the case where a distribution has equal-sized right and left tails, it is **symmetric**. The mean is approximately **equal** to the median. Think of mean as the balancing point of the distribution.

```
sns.histplot(data = wb, x = 'Access to an improved water source: % of population: 2015', stat = 'density')
plt.title('Distribution with a long left tail')
```

Text(0.5, 1.0, 'Distribution with a long left tail')



#### 7.6.3.3.2 Outliers

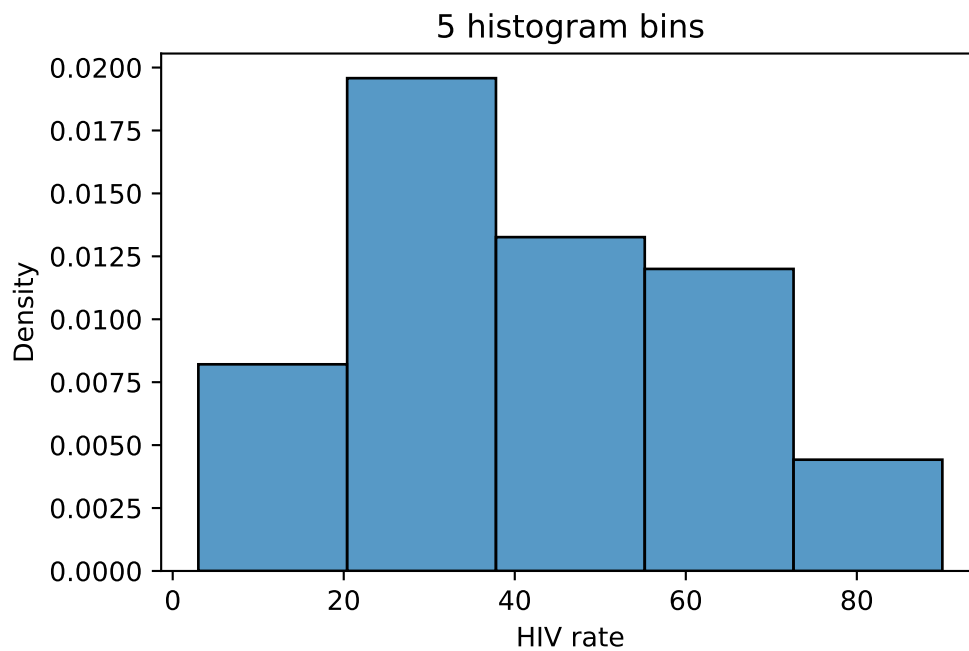
Loosely speaking, an **outlier** is defined as a data point that lies an abnormally large distance away from other values. Let's make this more concrete. As you may have observed in the box plot infographic earlier, we define **outliers** to be the data points that fall beyond the whiskers. Specifically, values that are less than the [ $1^{st}$  Quartile  $- (1.5 \times \text{IQR})$ ], or greater than [ $3^{rd}$  Quartile  $+ (1.5 \times \text{IQR})$ ].

#### 7.6.3.3.3 Modes

In Data 100, we describe a “mode” of a histogram as a peak in the distribution. Often, however, it is difficult to determine what counts as its own “peak.” For example, the number of peaks in the distribution of HIV rates across different countries varies depending on the number of histogram bins we plot.

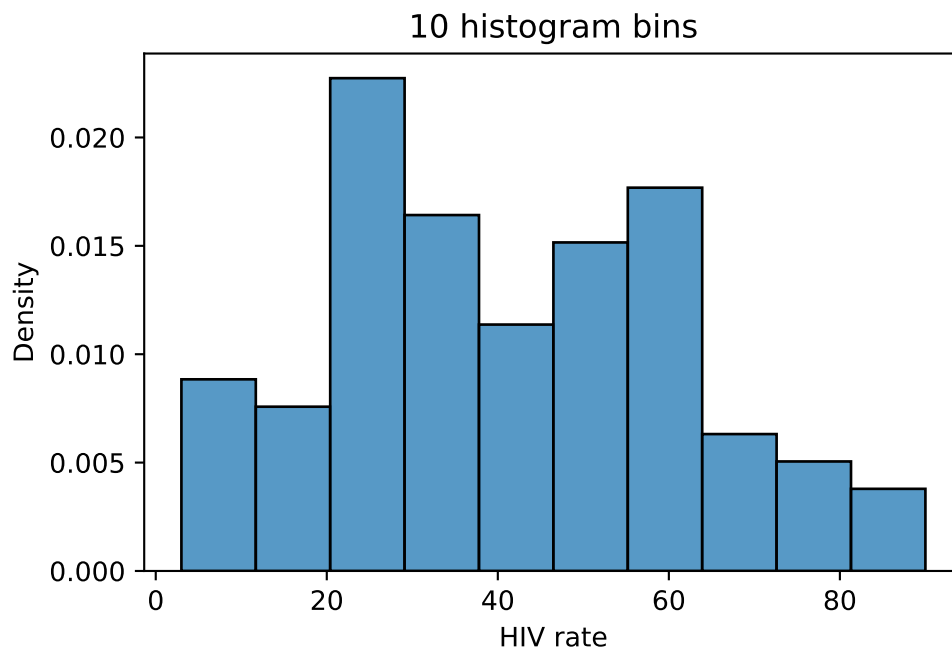
If we set the number of bins to 5, the distribution appears unimodal.

```
# Rename the very long column name for convenience
wb = wb.rename(columns={'Antiretroviral therapy coverage: % of people living with HIV: 2015'})
# With 5 bins, it seems that there is only one peak
sns.histplot(data=wb, x="HIV rate", stat="density", bins=5)
plt.title("5 histogram bins");
```



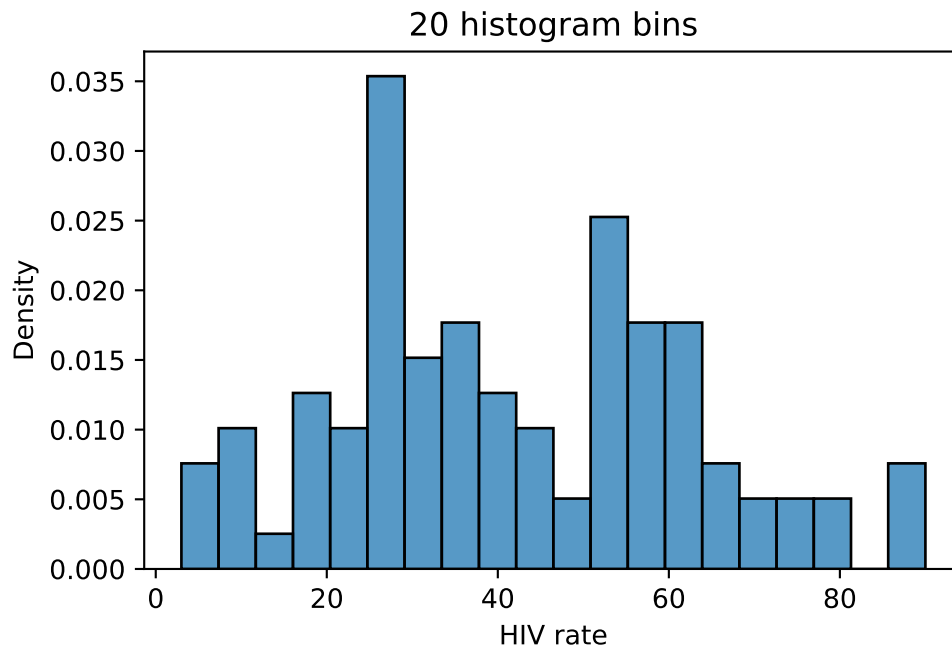
```
# With 10 bins, there seem to be two peaks
```

```
sns.histplot(data=wb, x="HIV rate", stat="density", bins=10)  
plt.title("10 histogram bins");
```



```
# And with 20 bins, it becomes hard to say what counts as a "peak"!
```

```
sns.histplot(data=wb, x="HIV rate", stat="density", bins=20)  
plt.title("20 histogram bins");
```



In part, it is these ambiguities that motivate us to consider using Kernel Density Estimation (KDE), which we will explore more in the next lecture.

## 8 Visualization II

### **i** Learning Outcomes

- Understanding KDE for plotting distributions and estimating density curves.
- Using transformations to analyze the relationship between two variables.
- Evaluating the quality of a visualization based on visualization theory concepts.

### 8.1 Kernel Density Estimation

Often, we want to identify general trends across a distribution, rather than focus on detail. Smoothing a distribution helps generalize the structure of the data and eliminate noise.

#### 8.1.1 KDE Theory

A **kernel density estimate (KDE)** is a smooth, continuous function that approximates a curve. It allows us to represent general trends in a distribution without focusing on the details, which is useful for analyzing the broad structure of a dataset.

More formally, a KDE attempts to approximate the underlying **probability distribution** from which our dataset was drawn. You may have encountered the idea of a probability distribution in your other classes; if not, we'll discuss it at length in the next lecture. For now, you can think of a probability distribution as a description of how likely it is for us to sample a particular value in our dataset.

A KDE curve estimates the probability density function of a random variable. Consider the example below, where we have used `sns.displot` to plot both a histogram (containing the data points we actually collected) and a KDE curve (representing the *approximated* probability distribution from which this data was drawn) using data from the World Bank dataset (`wb`).

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import warnings
```

```
warnings.filterwarnings("ignore", "use_inf_as_na") # Supresses distracting deprecation warnin

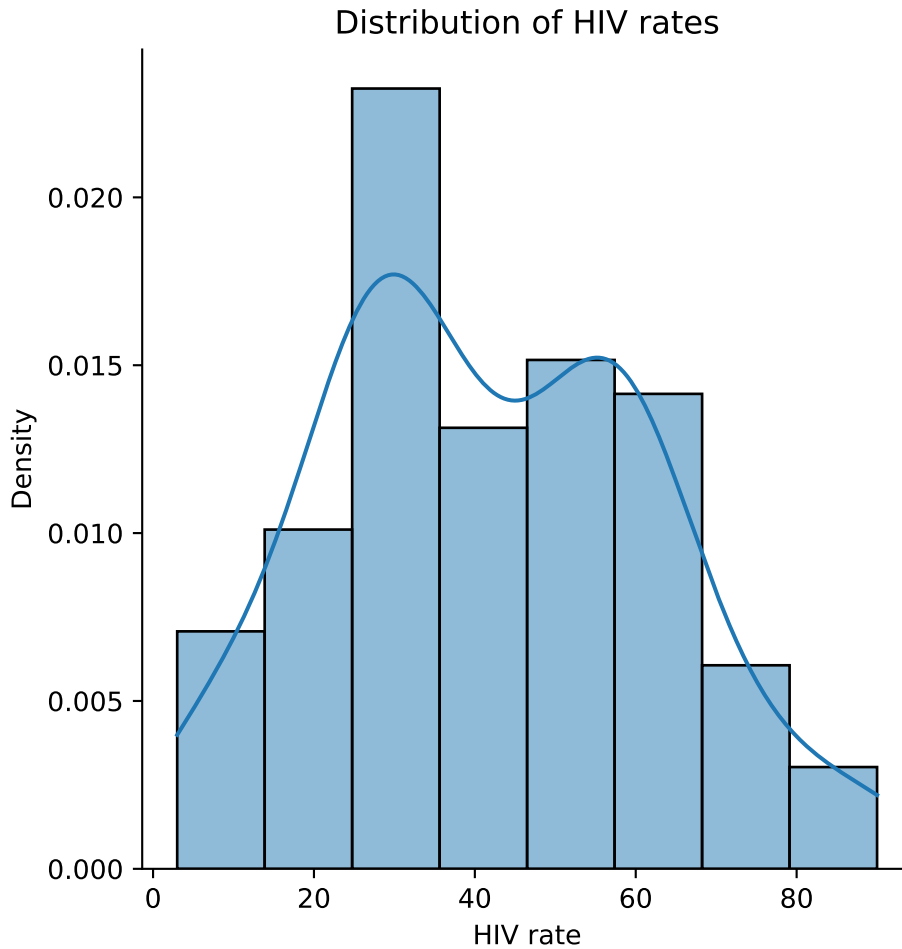
wb = pd.read_csv("data/world_bank.csv", index_col=0)
wb = wb.rename(columns={'Antiretroviral therapy coverage: % of people living with HIV: 2015': 'hiv_rate',
                        'Gross national income per capita, Atlas method: $: 2016': 'gni'})
wb.head()
```

	Continent	Country	Primary completion rate: Male: % of relevant age group: 2015	Primary completion
0	Africa	Algeria	106.0	105.0
1	Africa	Angola	NaN	NaN
2	Africa	Benin	83.0	73.0
3	Africa	Botswana	98.0	101.0
5	Africa	Burundi	58.0	66.0

```
import seaborn as sns
import matplotlib.pyplot as plt

sns.displot(data = wb, x = 'HIV rate', \
            kde = True, stat = "density")

plt.title("Distribution of HIV rates");
```



Notice that the smooth KDE curve is higher when the histogram bins are taller. You can think of the height of the KDE curve as representing how “probable” it is that we randomly sample a datapoint with the corresponding value. This intuitively makes sense – if we have already collected more datapoints with a particular value (resulting in a tall histogram bin), it is more likely that, if we randomly sample another datapoint, we will sample one with a similar value (resulting in a high KDE curve).

The area under a probability density function should always integrate to 1, representing the fact that the total probability of a distribution should always sum to 100%. Hence, a KDE curve will always have an area under the curve of 1.

### 8.1.2 Constructing a KDE

We perform kernel density estimation using three steps.



1. Place a kernel at each datapoint.
2. Normalize the kernels to have a total area of 1 (across all kernels).
3. Sum the normalized kernels.

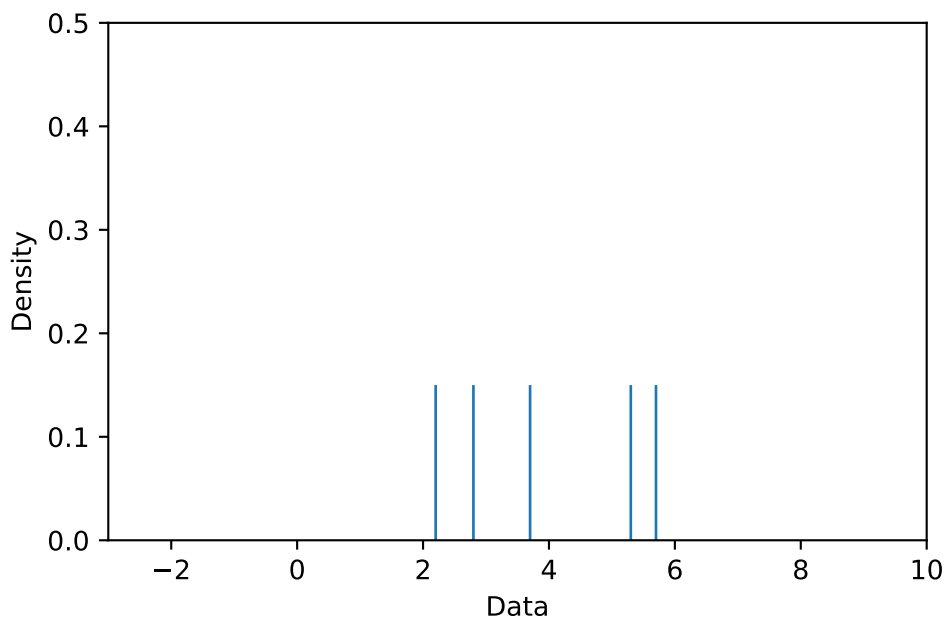
We'll explain what a "kernel" is momentarily.

To make things simpler, let's construct a KDE for a small, artificially generated dataset of 5 datapoints: [2.2, 2.8, 3.7, 5.3, 5.7]. In the plot below, each vertical bar represents one data point.

```
data = [2.2, 2.8, 3.7, 5.3, 5.7]

sns.rugplot(data, height=0.3)

plt.xlabel("Data")
plt.ylabel("Density")
plt.xlim(-3, 10)
plt.ylim(0, 0.5);
```

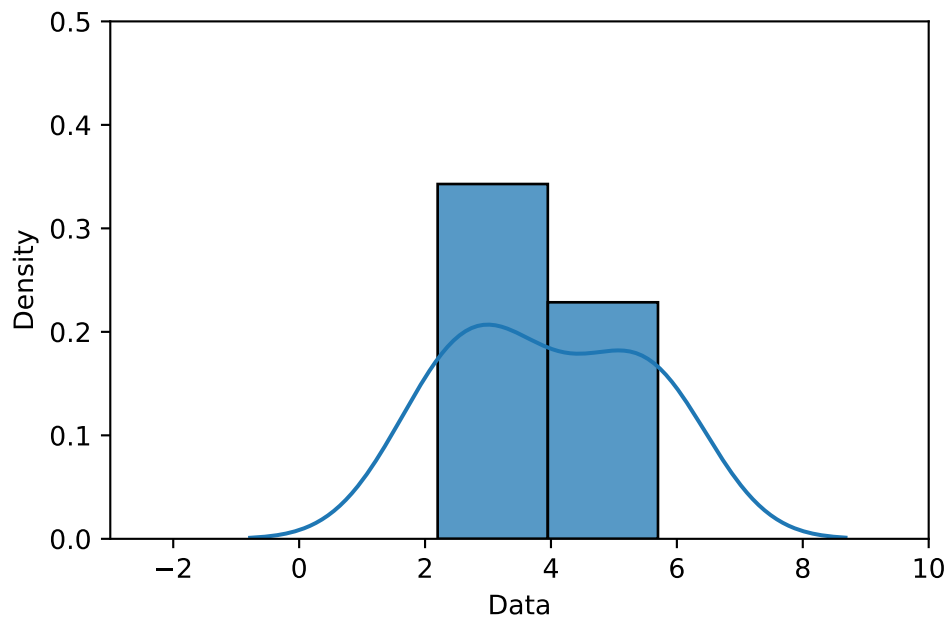


Our goal is to create the following KDE curve, which was generated automatically by `sns.kdeplot`.

```
plt.xlabel("Data")
plt.xlim(-3, 10)
```

```
plt.ylim(0, 0.5)

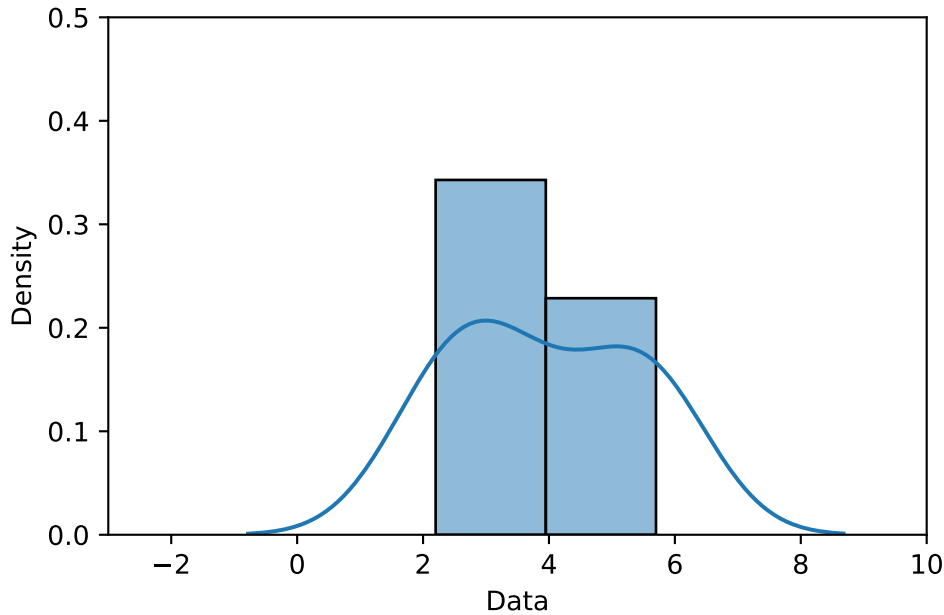
sns.kdeplot(data, bw_method=0.65)
sns.histplot(data, stat='density', bins=2);
```



Alternatively, we can use `sns.histplot`. You can also get a very similar result in a single call by requesting the KDE be added to the histogram, with `kde=True` and some extra keywords:

```
plt.xlabel("Data")
plt.xlim(-3, 10)
plt.ylim(0, 0.5)

sns.histplot(data, bins=2, kde=True, stat="density", kde_kws=dict(cut=3, bw_method=0.65));
```



#### 8.1.2.1 Step 1: Place a Kernel at Each Data Point

To begin generating a density curve, we need to choose a **kernel** and **bandwidth value** ( $\alpha$ ). What are these exactly?

A **kernel** is a density curve. It is the mathematical function that attempts to capture the randomness of each data point in our sampled data. To explain what this means, consider just *one* of the datapoints in our dataset: 2.2. We obtained this datapoint by randomly sampling some information out in the real world (you can imagine 2.2 as representing a single measurement taken in an experiment, for example). If we were to sample a new datapoint, we may obtain a slightly different value. It could be higher than 2.2; it could also be lower than 2.2. We make the assumption that any future sampled datapoints will likely be similar in value to the data we've already drawn. This means that our *kernel* – our description of the probability of randomly sampling any new value – will be greatest at the datapoint we've already drawn but still have non-zero probability above and below it. The area under any kernel should integrate to 1, representing the total probability of drawing a new datapoint.

A **bandwidth value**, usually denoted by  $\alpha$ , represents the width of the kernel. A large value of  $\alpha$  will result in a wide, short kernel function, while a small value will result in a narrow, tall kernel.

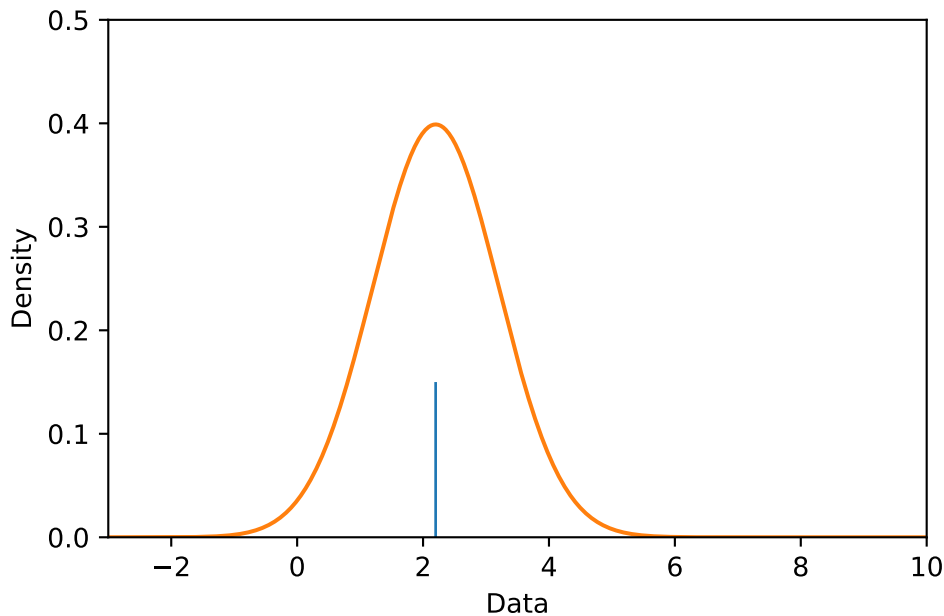
Below, we place a **Gaussian kernel**, plotted in orange, over the datapoint 2.2. A Gaussian kernel is simply the normal distribution, which you may have called a bell curve in Data 8.

```
def gaussian_kernel(x, z, a):
    # We'll discuss where this mathematical formulation came from later
    return (1/np.sqrt(2*np.pi*a**2)) * np.exp(-(x - z)**2 / (2 * a**2))

# Plot our datapoint
sns.rugplot([2.2], height=0.3)

# Plot the kernel
x = np.linspace(-3, 10, 1000)
plt.plot(x, gaussian_kernel(x, 2.2, 1))

plt.xlabel("Data")
plt.ylabel("Density")
plt.xlim(-3, 10)
plt.ylim(0, 0.5);
```



To begin creating our KDE, we place a kernel on *each* datapoint in our dataset. For our dataset of 5 points, we will have 5 kernels.

```
# You will work with the functions below in Lab 4
def create_kde(kernel, pts, a):
    # Takes in a kernel, set of points, and alpha
    # Returns the KDE as a function
```

```

def f(x):
    output = 0
    for pt in pts:
        output += kernel(x, pt, a)
    return output / len(pts) # Normalization factor
return f

def plot_kde(kernel, pts, a):
    # Calls create_kde and plots the corresponding KDE
    f = create_kde(kernel, pts, a)
    x = np.linspace(min(pts) - 5, max(pts) + 5, 1000)
    y = [f(xi) for xi in x]
    plt.plot(x, y);

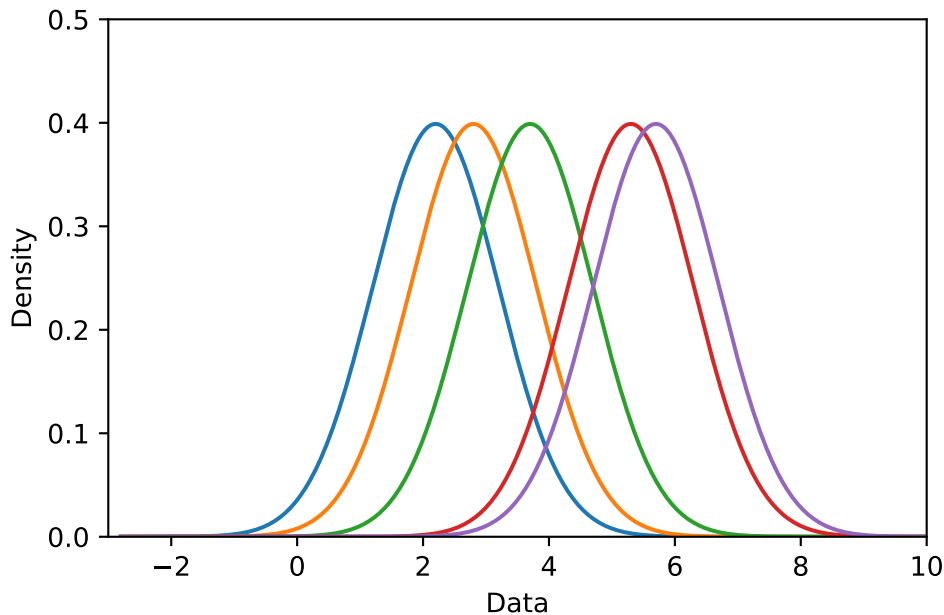
def plot_separate_kernels(kernel, pts, a, norm=False):
    # Plots individual kernels, which are then summed to create the KDE
    x = np.linspace(min(pts) - 5, max(pts) + 5, 1000)
    for pt in pts:
        y = kernel(x, pt, a)
        if norm:
            y /= len(pts)
        plt.plot(x, y)

    plt.show();

plt.xlim(-3, 10)
plt.ylim(0, 0.5)
plt.xlabel("Data")
plt.ylabel("Density")

plot_separate_kernels(gaussian_kernel, data, a = 1)

```



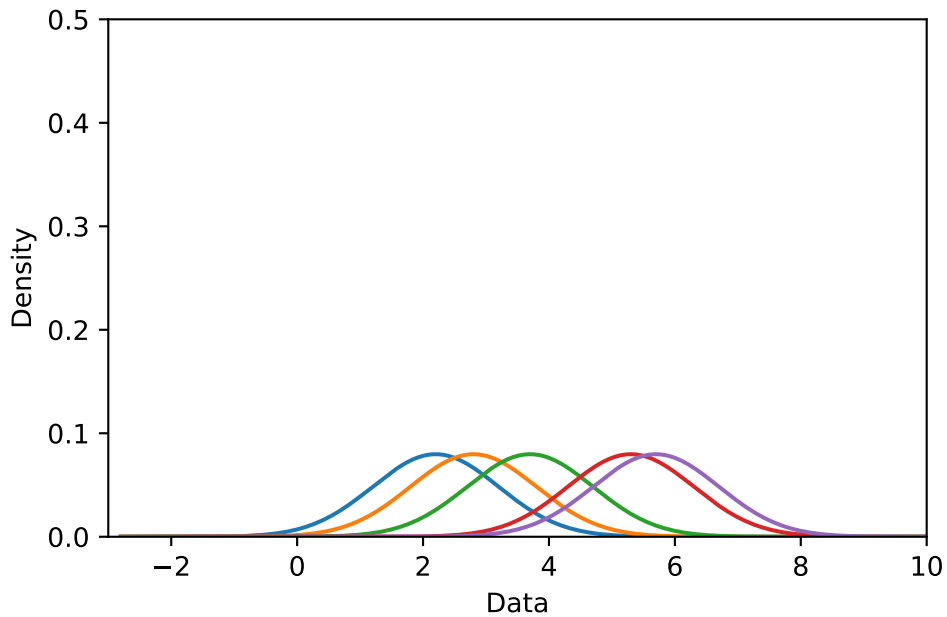
#### 8.1.2.2 Step 2: Normalize Kernels to Have a Total Area of 1

Above, we said that *each* kernel has an area of 1. Earlier, we also said that our goal is to construct a KDE curve using these kernels with a *total* area of 1. If we were to directly sum the kernels as they are, we would produce a KDE curve with an integrated area of (5 kernels)  $\times$  (area of 1 each) = 5. To avoid this, we will **normalize** each of our kernels. This involves multiplying each kernel by  $\frac{1}{\text{\# datapoints}}$ .

In the cell below, we multiply each of our 5 kernels by  $\frac{1}{5}$  to apply normalization.

```
plt.xlim(-3, 10)
plt.ylim(0, 0.5)
plt.xlabel("Data")
plt.ylabel("Density")

# The `norm` argument specifies whether or not to normalize the kernels
plot_separate_kernels(gaussian_kernel, data, a = 1, norm = True)
```

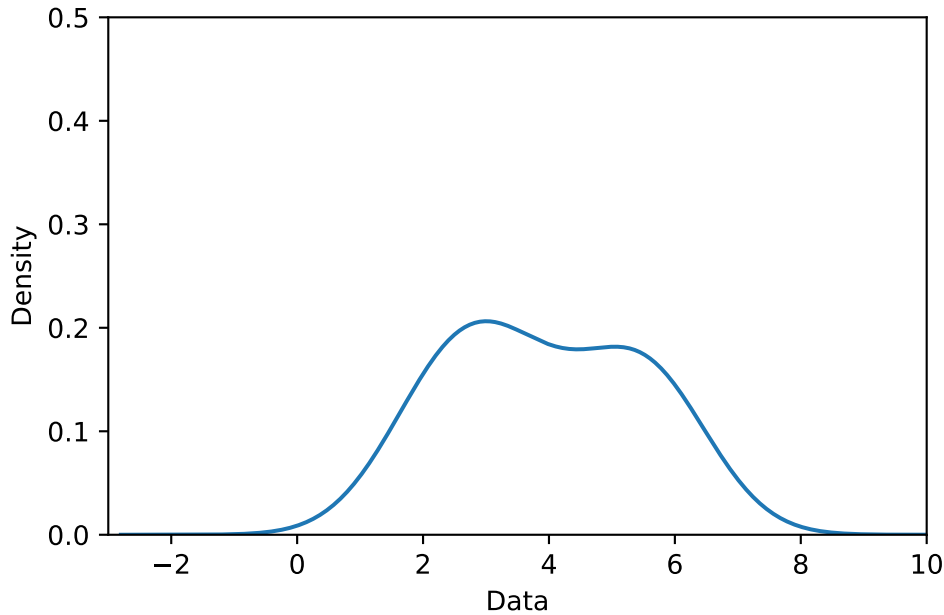


### 8.1.2.3 Step 3: Sum the Normalized Kernels

Our KDE curve is the sum of the normalized kernels. Notice that the final curve is identical to the plot generated by `sns.kdeplot` we saw earlier!

```
plt.xlim(-3, 10)
plt.ylim(0, 0.5)
plt.xlabel("Data")
plt.ylabel("Density")

plot_kde(gaussian_kernel, data, a=1)
```



### 8.1.3 Kernel Functions and Bandwidths

A general “KDE formula” function is given above.

1.  $K_\alpha(x, x_i)$  is the kernel centered on the observation  $i$ .
  - Each kernel individually has area 1.
  - $x$  represents any number on the number line. It is the input to our function.
2.  $n$  is the number of observed datapoints that we have.
  - We multiply by  $\frac{1}{n}$  so that the total area of the KDE is still 1.
3. Each  $x_i \in \{x_1, x_2, \dots, x_n\}$  represents an observed datapoint.
  - These are what we use to create our KDE by summing multiple shifted kernels centered at these points.
  - $\alpha$  (alpha) is the bandwidth or smoothing parameter.

A **kernel** (for our purposes) is a valid density function. This means it:

- Must be non-negative for all inputs.
- Must integrate to 1.



### 8.1.3.1 Gaussian Kernel

The most common kernel is the **Gaussian kernel**. The Gaussian kernel is equivalent to the Gaussian probability density function (the Normal distribution), centered at the observed value with a standard deviation of  $\alpha$  (this is known as the **bandwidth** parameter).

$$K_a(x, x_i) = \frac{1}{\sqrt{2\pi\alpha^2}} e^{-\frac{(x-x_i)^2}{2\alpha^2}}$$

In this formula:

- $x$  (no subscript) represents any value along the x-axis of our plot
- $x_i$  represents the  $i$ -th datapoint in our dataset. It is one of the values that we have actually collected in our data sampling process. In our example earlier,  $x_i = 2.2$ . Those of you who have taken a probability class may recognize  $x_i$  as the **mean** of the normal distribution.
- Each kernel is **centered** on our observed values, so its distribution mean is  $x_i$ .
- $\alpha$  is the bandwidth parameter, representing the width of our kernel. More formally,  $\alpha$  is the **standard deviation** of the Gaussian curve.
  - A large value of  $\alpha$  will produce a kernel that is wider and shorter – this leads to a smoother KDE when the kernels are summed together.
  - A small value of  $\alpha$  will produce a narrower, taller kernel, and, with it, a noisier KDE.

The details of this (admittedly intimidating) formula are less important than understanding its role in kernel density estimation – this equation gives us the shape of each kernel.

---

Gaussian Kernel,  $\alpha = 0.1$

Gaussian Kernel,  $\alpha = 1$

---

---

Gaussian Kernel,  $\alpha = 2$

Gaussian Kernel,  $\alpha = 5$

---

### 8.1.3.2 Boxcar Kernel

Another example of a kernel is the **Boxcar kernel**. The boxcar kernel assigns a uniform density to points within a “window” of the observation, and a density of 0 elsewhere. The equation below is a boxcar kernel with the center at  $x_i$  and the bandwidth of  $\alpha$ .

$$K_a(x, x_i) = \begin{cases} \frac{1}{\alpha}, & |x - x_i| \leq \frac{\alpha}{2} \\ 0, & \text{else} \end{cases}$$

The boxcar kernel is seldom used in practice – we include it here to demonstrate that a kernel function can take whatever form you would like, provided it integrates to 1 and does not output negative values.

```
def boxcar_kernel(alpha, x, z):
    return (((x-z)>=-alpha/2)&((x-z)<=alpha/2))/alpha

xs = np.linspace(-5, 5, 200)
alpha=1
kde_curve = [boxcar_kernel(alpha, x, 0) for x in xs]
plt.plot(xs, kde_curve);
```

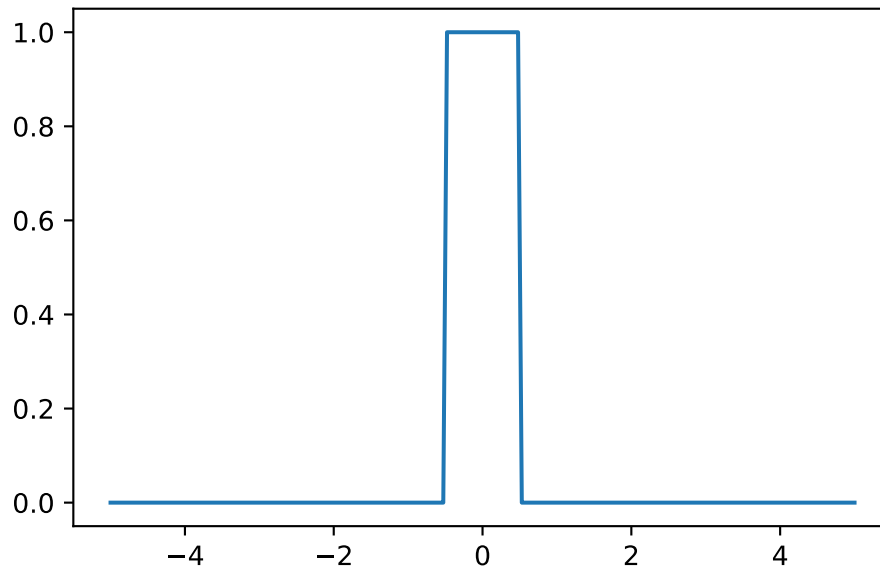


Figure 8.1: The Boxcar kernel centered at 0 with bandwidth  $\alpha = 1$ .

The diagram on the right is how the density curve for our 5 point dataset would have looked had we used the Boxcar kernel with bandwidth  $\alpha = 1$ .

KDE	Boxcar

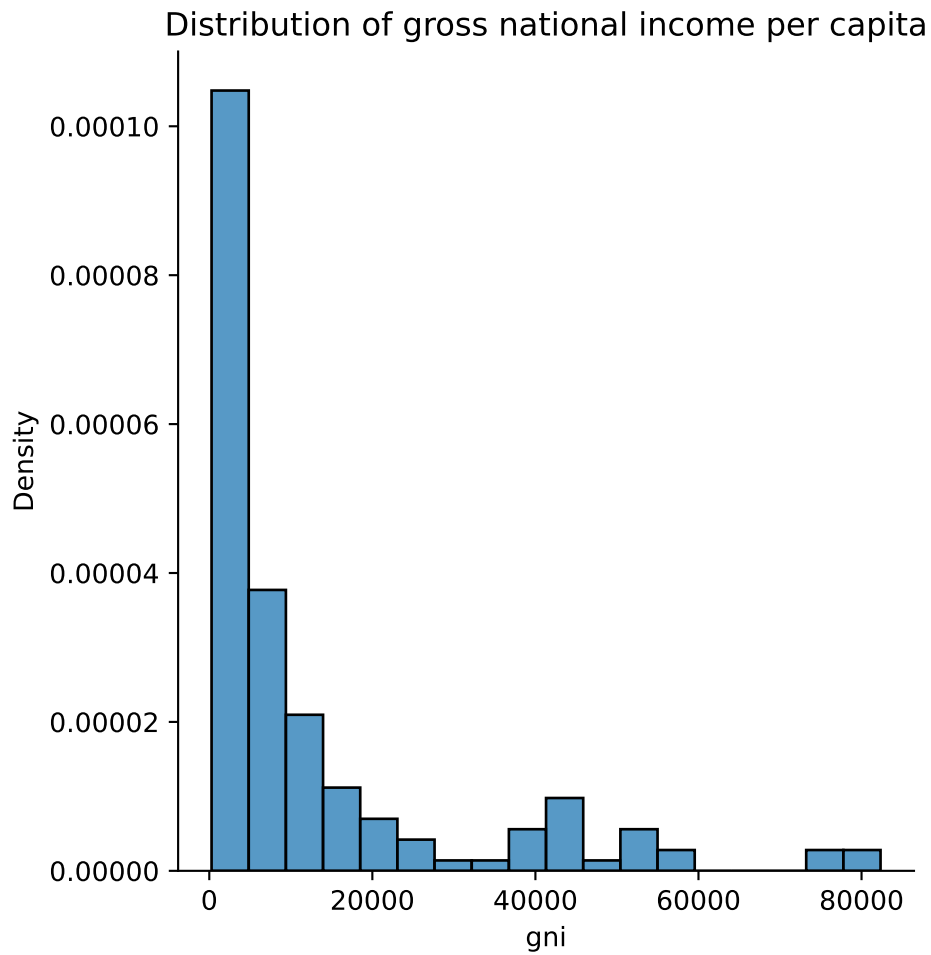
## 8.2 Diving Deeper into displot

As we saw earlier, we can use `seaborn`'s `displot` function to plot various distributions. In particular, `displot` allows you to specify the kind of plot and is a wrapper for `histplot`, `kdeplot`, and `ecdfplot`.

Below, we can see a couple of examples of how `sns.displot` can be used to plot various distributions.

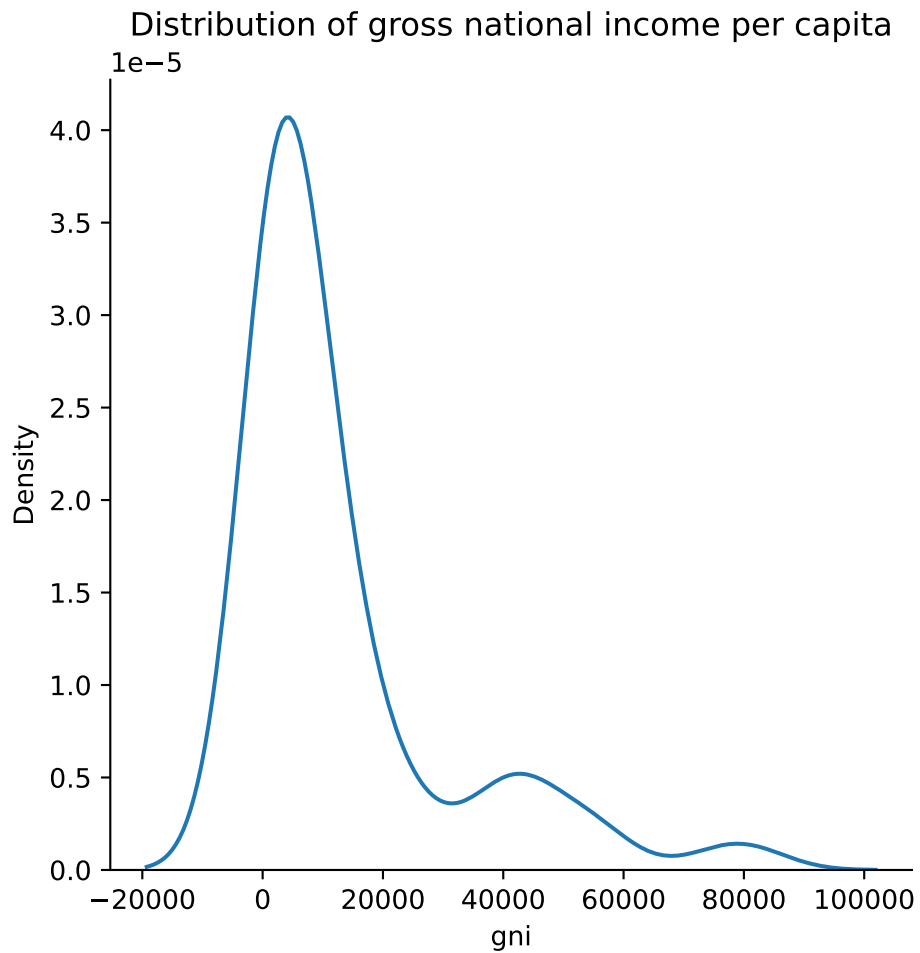
First, we can plot a histogram by setting `kind` to `"hist"`. Note that here we've specified `stat = density` to normalize the histogram such that the area under the histogram is equal to 1.

```
sns.displot(data=wb,
            x="gni",
            kind="hist",
            stat="density") # default: stat=count and density integrates to 1
plt.title("Distribution of gross national income per capita");
```



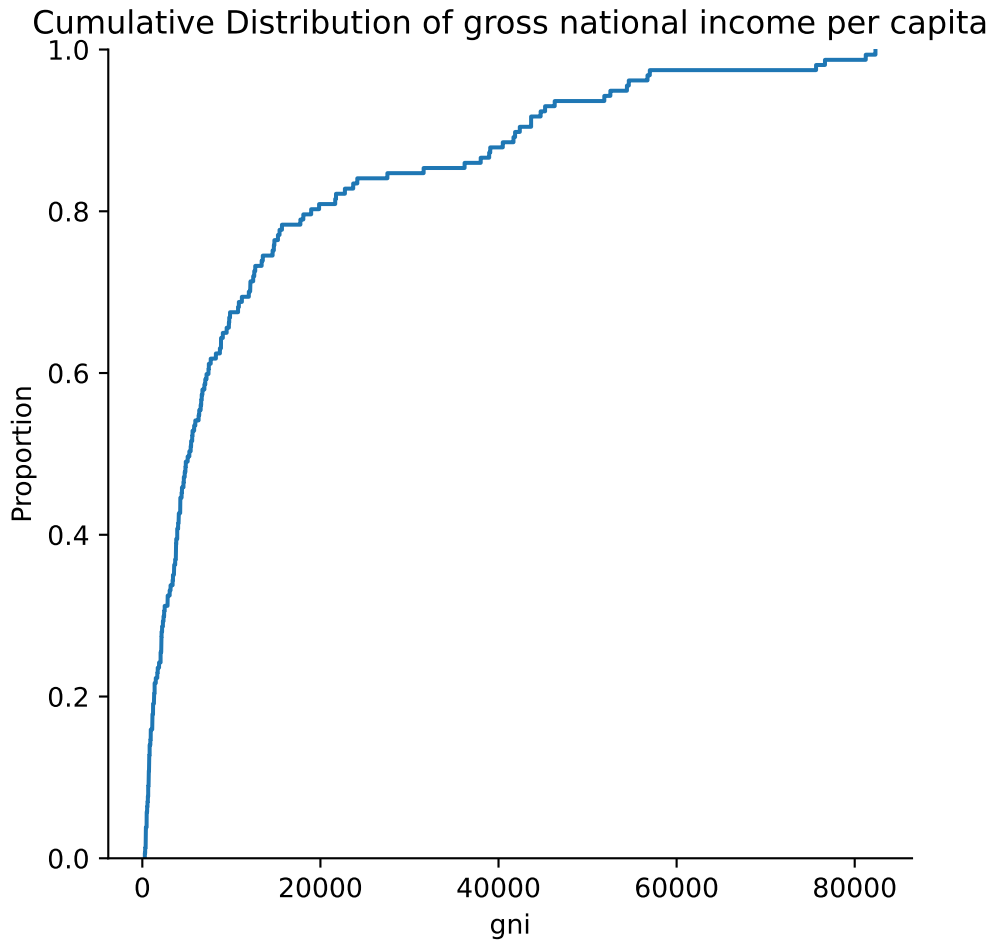
Now, what if we want to generate a KDE plot? We can set `kind = "kde"`!

```
sns.displot(data=wb,  
            x="gni",  
            kind='kde')  
plt.title("Distribution of gross national income per capita");
```



And finally, if we want to generate an Empirical Cumulative Distribution Function (ECDF), we can specify `kind = "ecdf"`.

```
sns.displot(data=wb,  
            x="gni",  
            kind='ecdf')  
plt.title("Cumulative Distribution of gross national income per capita");
```



## 8.3 Relationships Between Quantitative Variables

Up until now, we've discussed how to visualize single-variable distributions. Going beyond this, we want to understand the relationship between pairs of numerical variables.

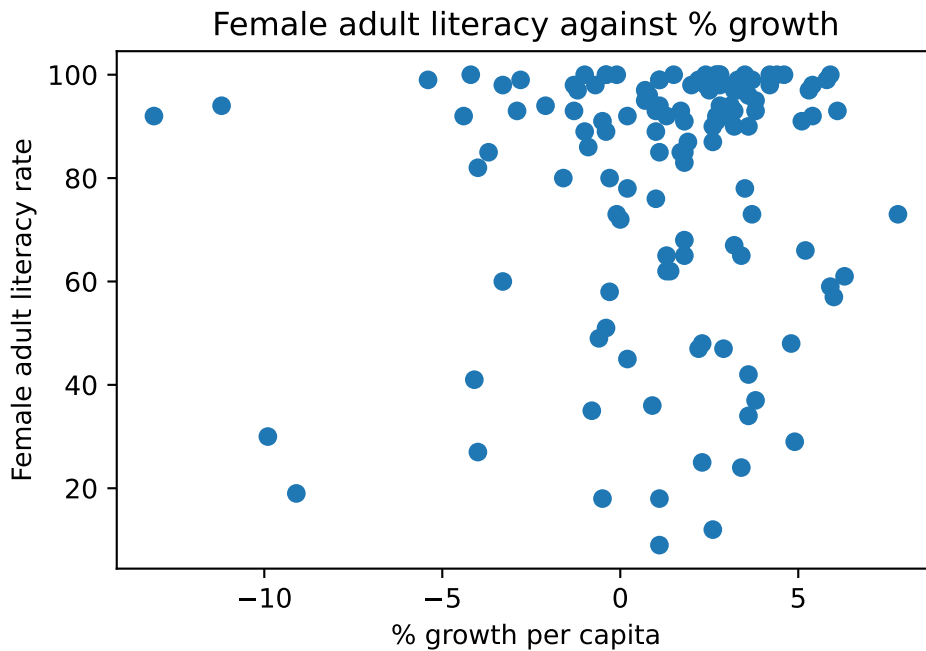
### 8.3.0.1 Scatter Plots

**Scatter plots** are one of the most useful tools in representing the relationship between **pairs** of quantitative variables. They are particularly important in gauging the strength, or correlation, of the relationship between variables. Knowledge of these relationships can then motivate decisions in our modeling process.

In `matplotlib`, we use the function `plt.scatter` to generate a scatter plot. Notice that, unlike our examples of plotting single-variable distributions, now we specify sequences of values to be plotted along the x-axis *and* the y-axis.

```
plt.scatter(wb["per capita: % growth: 2016"], \
            wb['Adult literacy rate: Female: % ages 15 and older: 2005-14'])

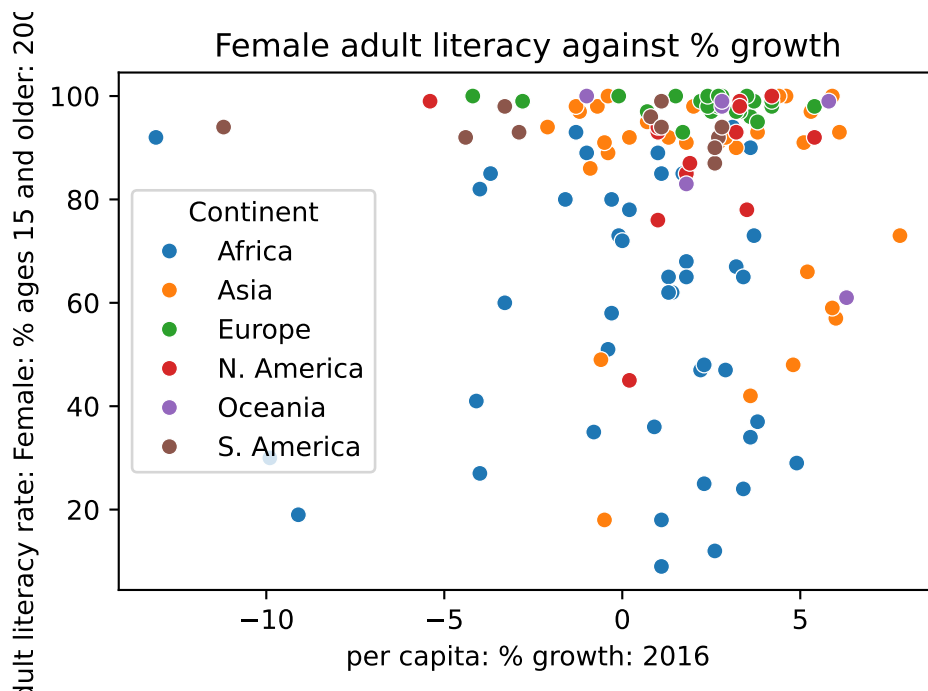
plt.xlabel("% growth per capita")
plt.ylabel("Female adult literacy rate")
plt.title("Female adult literacy against % growth");
```



In `seaborn`, we call the function `sns.scatterplot`. We use the `x` and `y` parameters to indicate the values to be plotted along the x and y axes, respectively. By using the `hue` parameter, we can specify a third variable to be used for coloring each scatter point.

```
sns.scatterplot(data = wb, x = "per capita: % growth: 2016", \
                y = "Adult literacy rate: Female: % ages 15 and older: 2005-14",
                hue = "Continent")

plt.title("Female adult literacy against % growth");
```



#### 8.3.0.1.1 Overplotting

Although the plots above communicate the general relationship between the two plotted variables, they both suffer a major limitation – **overplotting**. Overplotting occurs when scatter points with similar values are stacked on top of one another, making it difficult to see the number of scatter points actually plotted in the visualization. Notice how in the upper right-hand region of the plots, we cannot easily tell just how many points have been plotted. This makes our visualizations difficult to interpret.

We have a few methods to help reduce overplotting:

- Decreasing the size of the scatter point markers can improve readability. We do this by setting a new value to the size parameter, `s`, of `plt.scatter` or `sns.scatterplot`.
- **Jittering** is the process of adding a small amount of random noise to all x and y values to slightly shift the position of each datapoint. By randomly shifting all the data by some small distance, we can discern individual points more clearly without modifying the major trends of the original dataset.

In the cell below, we first jitter the data using `np.random.uniform`, then re-plot it with smaller markers. The resulting plot is much easier to interpret.

```
# Setting a seed ensures that we produce the same plot each time
# This means that the course notes will not change each time you access them
```



```

np.random.seed(150)

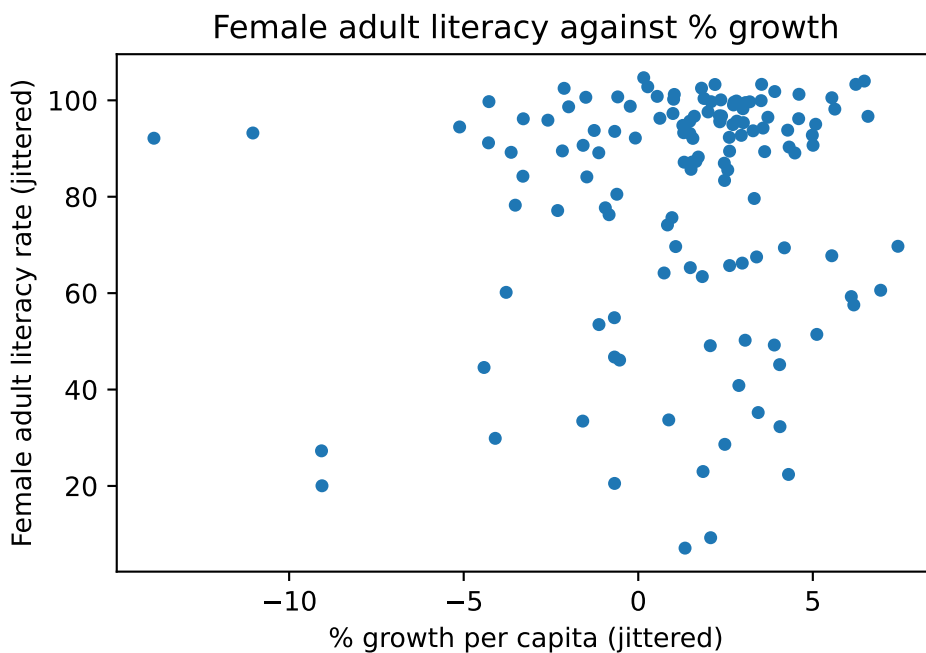
# This call to np.random.uniform generates random numbers between -1 and 1
# We add these random numbers to the original x data to jitter it slightly
x_noise = np.random.uniform(-1, 1, len(wb))
jittered_x = wb["per capita: % growth: 2016"] + x_noise

# Repeat for y data
y_noise = np.random.uniform(-5, 5, len(wb))
jittered_y = wb["Adult literacy rate: Female: % ages 15 and older: 2005-14"] + y_noise

# Setting the size parameter `s` changes the size of each point
plt.scatter(jittered_x, jittered_y, s=15)

plt.xlabel("% growth per capita (jittered)")
plt.ylabel("Female adult literacy rate (jittered)")
plt.title("Female adult literacy against % growth");

```



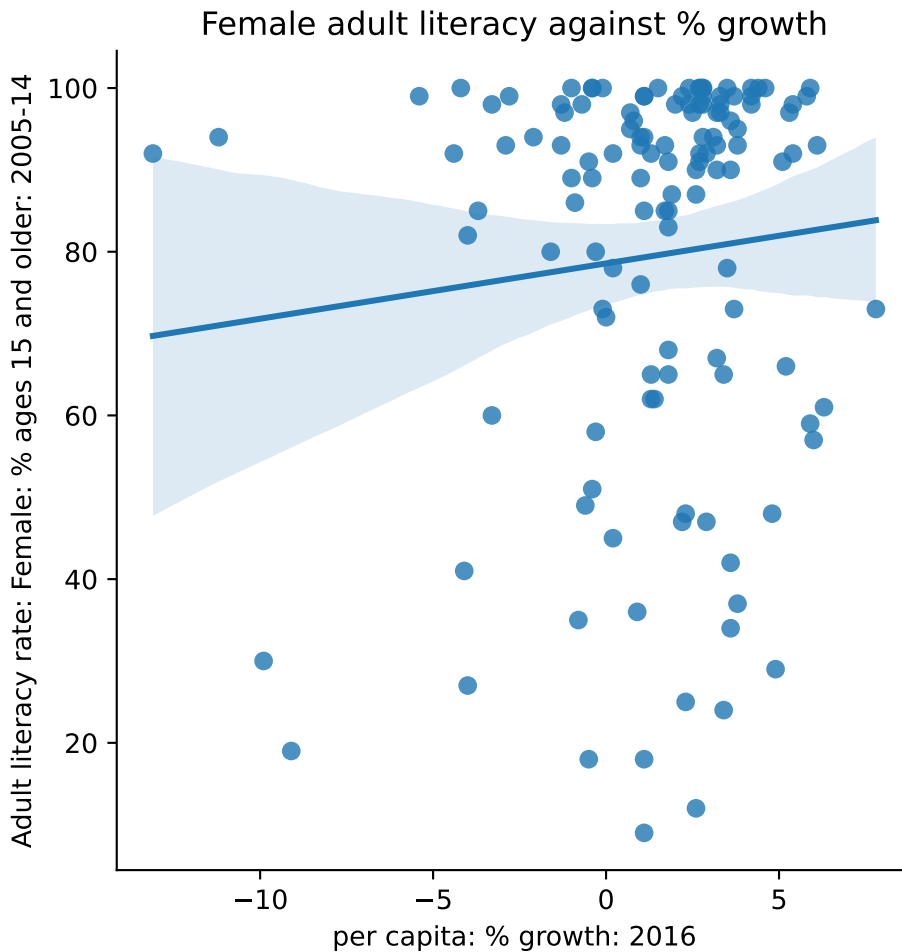
### 8.3.0.2 lmpplot and jointplot

seaborn also includes several built-in functions for creating more sophisticated scatter plots. Two of the most commonly used examples are `sns.lmpplot` and `sns.jointplot`.

`sns.lmplot` plots both a scatter plot *and* a linear regression line, all in one function call. We'll discuss linear regression in a few lectures.

```
sns.lmplot(data = wb, x = "per capita: % growth: 2016", \
           y = "Adult literacy rate: Female: % ages 15 and older: 2005-14")

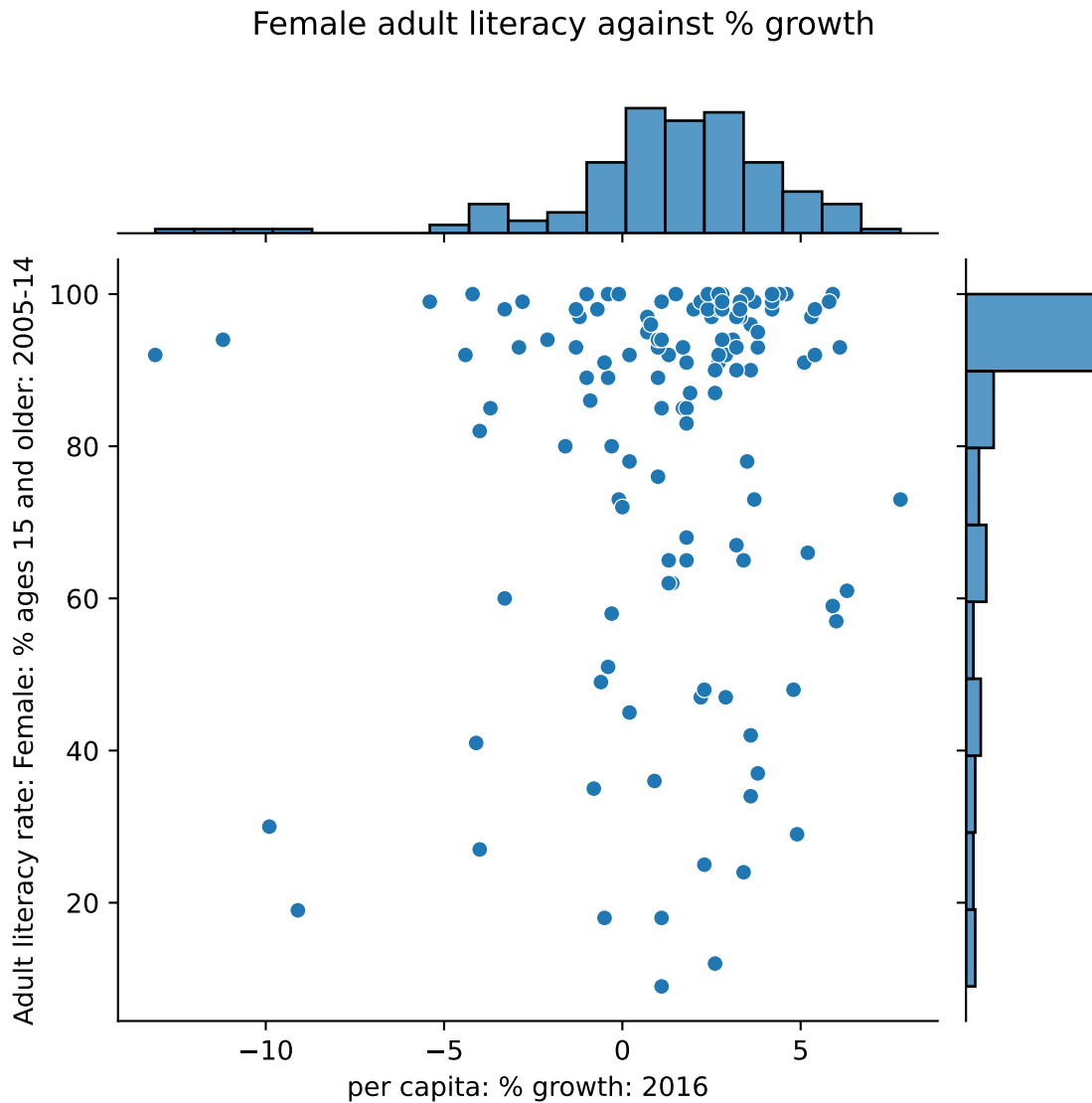
plt.title("Female adult literacy against % growth");
```



`sns.jointplot` creates a visualization with three components: a scatter plot, a histogram of the distribution of x values, and a histogram of the distribution of y values.

```
sns.jointplot(data = wb, x = "per capita: % growth: 2016", \
              y = "Adult literacy rate: Female: % ages 15 and older: 2005-14")
```

```
# plt.suptitle allows us to shift the title up so it does not overlap with the histogram
plt.suptitle("Female adult literacy against % growth")
plt.subplots_adjust(top=0.9);
```



### 8.3.0.3 Hex plots

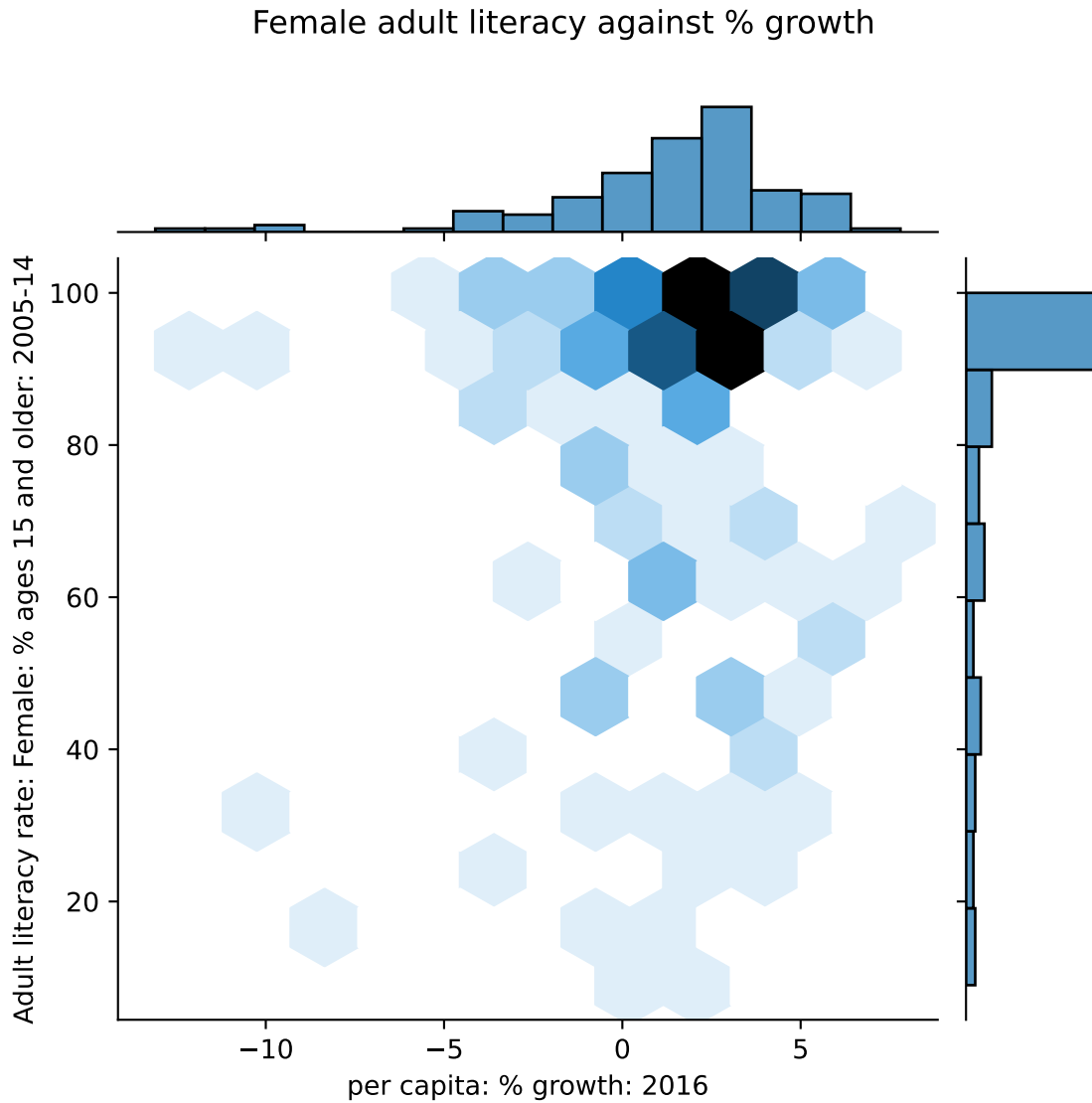
For datasets with a very large number of datapoints, jittering is unlikely to fully resolve the issue of overplotting. In these cases, we can attempt to visualize our data by its *density*, rather than displaying each individual datapoint.

**Hex plots** can be thought of as two-dimensional histograms that show the joint distribution between two variables. This is particularly useful when working with very dense data. In a hex plot, the x-y plane is binned into hexagons. Hexagons that are darker in color indicate a greater density of data – that is, there are more data points that lie in the region enclosed by the hexagon.

We can generate a hex plot using `sns.jointplot` modified with the `kind` parameter.

```
sns.jointplot(data = wb, x = "per capita: % growth: 2016", \
              y = "Adult literacy rate: Female: % ages 15 and older: 2005-14", \
              kind = "hex")

# plt.suptitle allows us to shift the title up so it does not overlap with the histogram
plt.suptitle("Female adult literacy against % growth")
plt.subplots_adjust(top=0.9);
```



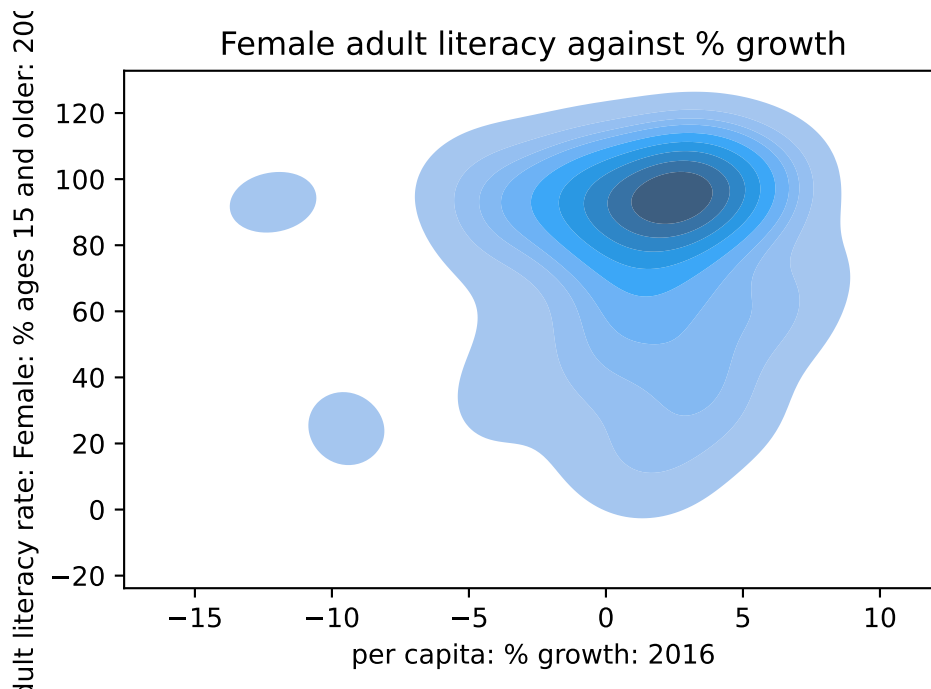
#### 8.3.0.4 Contour Plots

**Contour plots** are an alternative way of plotting the joint distribution of two variables. You can think of them as the 2-dimensional versions of KDE plots. A contour plot can be interpreted in a similar way to a [topographic map](#). Each contour line represents an area that has the same *density* of datapoints throughout the region. Contours marked with darker colors contain more datapoints (a higher density) in that region.

`sns.kdeplot` will generate a contour plot if we specify both x and y data.

```
sns.kdeplot(data = wb, x = "per capita: % growth: 2016", \
            y = "Adult literacy rate: Female: % ages 15 and older: 2005-14", \
            fill = True)

plt.title("Female adult literacy against % growth");
```



## 8.4 Transformations

We have now covered visualizations in great depth, looking into various forms of visualizations, plotting libraries, and high-level theory.

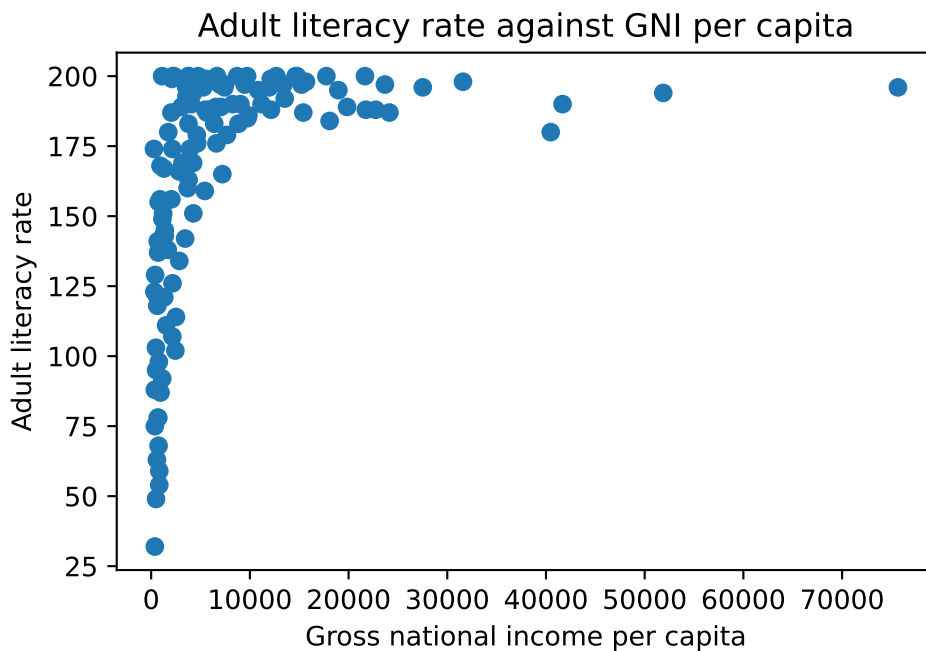
Much of this was done to uncover insights in data, which will prove necessary when we begin building models of data later in the course. A strong graphical correlation between two variables hints at an underlying relationship that we may want to study in greater detail. However, relying on visual relationships alone is limiting - not all plots show association. The presence of outliers and other statistical anomalies makes it hard to interpret data.

**Transformations** are the process of manipulating data to find significant relationships between variables. These are often found by applying mathematical functions to variables that “transform” their range of possible values and highlight some previously hidden associations between data.

To see why we may want to transform data, consider the following plot of adult literacy rates against gross national income.

```
# Some data cleaning to help with the next example
df = pd.DataFrame(index=wb.index)
df['lit'] = wb['Adult literacy rate: Female: % ages 15 and older: 2005-14'] \
            + wb["Adult literacy rate: Male: % ages 15 and older: 2005-14"]
df['inc'] = wb['gni']
df.dropna(inplace=True)

plt.scatter(df["inc"], df["lit"])
plt.xlabel("Gross national income per capita")
plt.ylabel("Adult literacy rate")
plt.title("Adult literacy rate against GNI per capita");
```



This plot is difficult to interpret for two reasons:

- The data shown in the visualization appears almost “smushed” – it is heavily concentrated in the upper lefthand region of the plot. Even if we jittered the dataset, we likely would not be able to fully assess all datapoints in that area.
- It is hard to generalize a clear relationship between the two plotted variables. While adult literacy rate appears to share some positive relationship with gross national income, we are not able to describe the specifics of this trend in much detail.

A transformation would allow us to visualize this data more clearly, which, in turn, would enable us to describe the underlying relationship between our variables of interest.

We will most commonly apply a transformation to **linearize a relationship** between variables. If we find a transformation to make a scatter plot of two variables linear, we can “backtrack” to find the exact relationship between the variables. This helps us in two major ways. Firstly, linear relationships are particularly simple to interpret – we have an intuitive sense of what the slope and intercept of a linear trend represent, and how they can help us understand the relationship between two variables. Secondly, linear relationships are the backbone of linear models. We will begin exploring linear modeling in great detail next week. As we’ll soon see, linear models become much more effective when we are working with linearized data.

In the remainder of this note, we will discuss how to linearize a dataset to produce the result below. Notice that the resulting plot displays a rough linear relationship between the values plotted on the x and y axes.

### 8.4.1 Linearization and Applying Transformations

To linearize a relationship, begin by asking yourself: what makes the data non-linear? It is helpful to repeat this question for each variable in your visualization.

Let’s start by considering the gross national income variable in our plot above. Looking at the y values in the scatter plot, we can see that many large y values are all clumped together, compressing the vertical axis. The scale of the horizontal axis is also being distorted by the few large outlying x values on the right.

If we decreased the size of these outliers relative to the bulk of the data, we could reduce the distortion of the horizontal axis. How can we do this? We need a transformation that will:

- Decrease the magnitude of large x values by a significant amount.
- Not drastically change the magnitude of small x values.

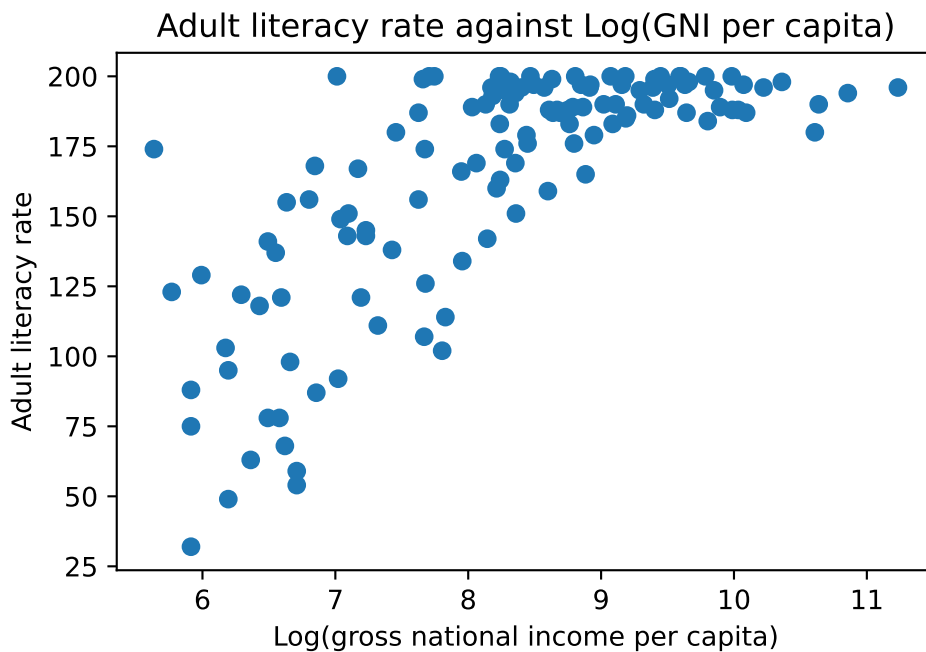
One function that produces this result is the **log transformation**. When we take the logarithm of a large number, the original number will decrease in magnitude dramatically. Conversely, when we take the logarithm of a small number, the original number does not change its value by as significant of an amount (to illustrate this, consider the difference between  $\log(100) = 4.61$  and  $\log(10) = 2.3$ ).

In Data 100 (and most upper-division STEM classes), log is used to refer to the natural logarithm with base  $e$ .



```
# np.log takes the logarithm of an array or Series
plt.scatter(np.log(df["inc"]), df["lit"])

plt.xlabel("Log(gross national income per capita)")
plt.ylabel("Adult literacy rate")
plt.title("Adult literacy rate against Log(GNI per capita)");
```



After taking the logarithm of our x values, our plot appears much more balanced in its horizontal scale. We no longer have many datapoints clumped on one end and a few outliers out at extreme values.

Let's repeat this reasoning for the y values. Considering only the vertical axis of the plot, notice how there are many datapoints concentrated at large y values. Only a few datapoints lie at smaller values of y.

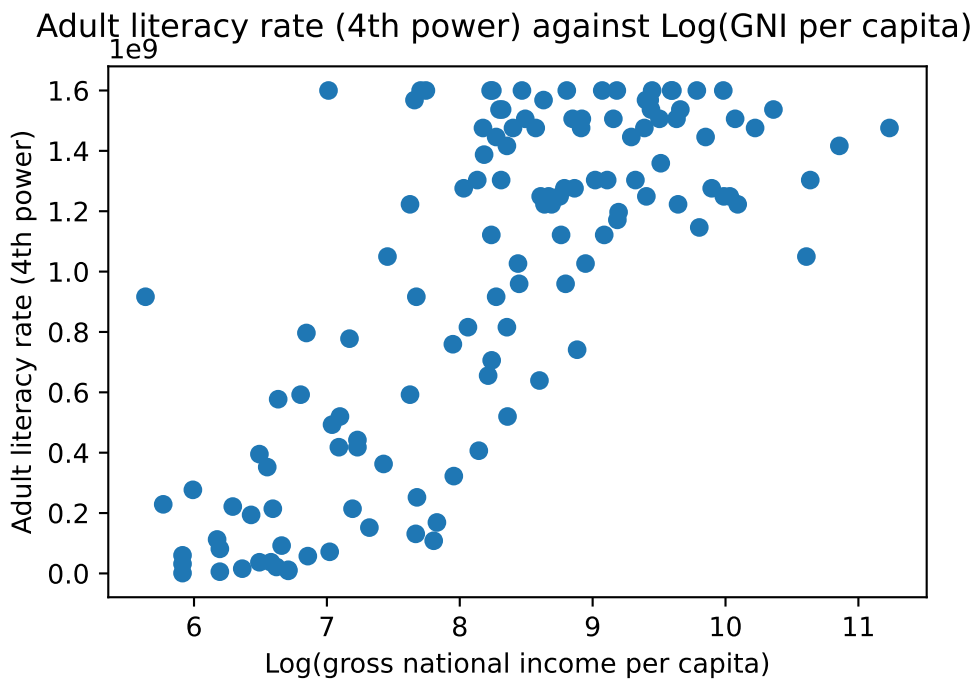
If we were to "spread out" these large values of y more, we would no longer see the dense concentration in one region of the y-axis. We need a transformation that will:

- Increase the magnitude of large values of y so these datapoints are distributed more broadly on the vertical scale,
- Not substantially alter the scaling of small values of y (we do not want to drastically modify the lower end of the y axis, which is already distributed evenly on the vertical scale).

In this case, it is helpful to apply a **power transformation** – that is, raise our y values to a power. Let's try raising our adult literacy rate values to the power of 4. Large values raised to the power of 4 will increase in magnitude proportionally much more than small values raised to the power of 4 (consider the difference between  $2^4 = 16$  and  $200^4 = 1600000000$ ).

```
# Apply a log transformation to the x values and a power transformation to the y values
plt.scatter(np.log(df["inc"]), df["lit"]**4)

plt.xlabel("Log(gross national income per capita)")
plt.ylabel("Adult literacy rate (4th power)")
plt.suptitle("Adult literacy rate (4th power) against Log(GNI per capita)")
plt.subplots_adjust(top=0.9);
```



Our scatter plot is looking a lot better! Now, we are plotting the log of our original x values on the horizontal axis, and the 4th power of our original y values on the vertical axis. We start to see an approximate *linear* relationship between our transformed variables.

What can we take away from this? We now know that the log of gross national income and adult literacy to the power of 4 are roughly linearly related. If we denote the original, untransformed gross national income values as  $x$  and the original adult literacy rate values as  $y$ , we can use the standard form of a linear fit to express this relationship:

$$y^4 = m(\log x) + b$$

Where  $m$  represents the slope of the linear fit, while  $b$  represents the intercept.

The cell below computes  $m$  and  $b$  for our transformed data. We'll discuss how this code was generated in a future lecture.

```
# The code below fits a linear regression model. We'll discuss it at length in a future lecture
from sklearn.linear_model import LinearRegression

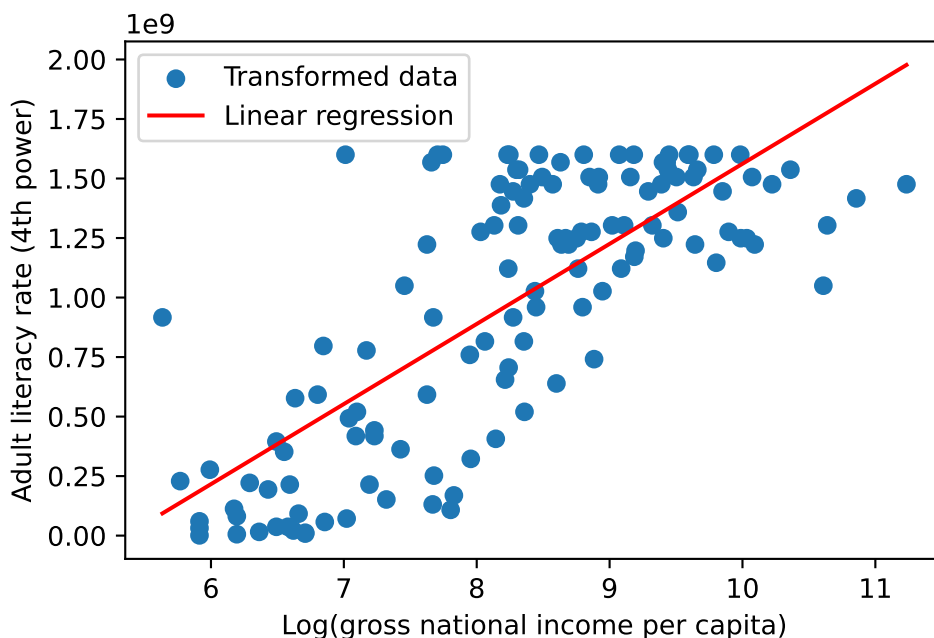
model = LinearRegression()
model.fit(np.log(df[["inc"]]), df["lit"]**4)
m, b = model.coef_[0], model.intercept_

print(f"The slope, m, of the transformed data is: {m}")
print(f"The intercept, b, of the transformed data is: {b}")

df = df.sort_values("inc")
plt.scatter(np.log(df["inc"]), df["lit"]**4, label="Transformed data")
plt.plot(np.log(df["inc"]), m*np.log(df["inc"])+b, c="red", label="Linear regression")
plt.xlabel("Log(gross national income per capita)")
plt.ylabel("Adult literacy rate (4th power)")
plt.legend();
```

The slope,  $m$ , of the transformed data is: 336400693.43172705

The intercept,  $b$ , of the transformed data is: -1802204836.0479987



What if we want to understand the *underlying* relationship between our original variables, before they were transformed? We can simply rearrange our linear expression above!

Recall our linear relationship between the transformed variables  $\log x$  and  $y^4$ .

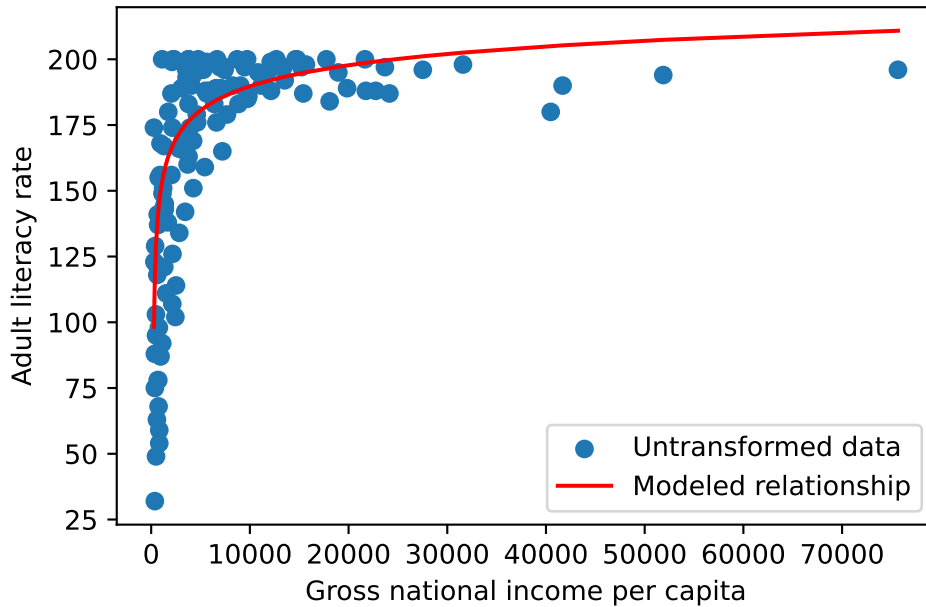
$$y^4 = m(\log x) + b$$

By rearranging the equation, we find a relationship between the untransformed variables  $x$  and  $y$ .

$$y = [m(\log x) + b]^{(1/4)}$$

When we plug in the values for  $m$  and  $b$  computed above, something interesting happens.

```
# Now, plug the values for m and b into the relationship between the untransformed x and y
plt.scatter(df["inc"], df["lit"], label="Untransformed data")
plt.plot(df["inc"], (m*np.log(df["inc"])+b)**(1/4), c="red", label="Modeled relationship")
plt.xlabel("Gross national income per capita")
plt.ylabel("Adult literacy rate")
plt.legend();
```



We have found a relationship between our original variables – gross national income and adult literacy rate!

Transformations are powerful tools for understanding our data in greater detail. To summarize what we just achieved:

- We identified appropriate transformations to **linearize** the original data.
- We used our knowledge of linear curves to compute the slope and intercept of the transformed data.
- We used this slope and intercept information to derive a relationship in the untransformed data.

Linearization will be an important tool as we begin our work on linear modeling next week.

#### 8.4.1.1 Tukey-Mosteller Bulge Diagram

The **Tukey-Mosteller Bulge Diagram** is a good guide when determining possible transformations to achieve linearity. It is a visual summary of the reasoning we just worked through above.

How does it work? Each curved “bulge” represents a possible shape of non-linear data. To use the diagram, find which of the four bulges resembles your dataset the most closely. Then, look at the axes of the quadrant for this bulge. The horizontal axis will list possible transformations that could be applied to your x data for linearization. Similarly, the vertical axis will list possible transformations that could be applied to your y data. Note that each axis

lists two possible transformations. While *either* of these transformations has the *potential* to linearize your dataset, note that this is an iterative process. It's important to try out these transformations and look at the results to see whether you've actually achieved linearity. If not, you'll need to continue testing other possible transformations.

Generally:

- $\sqrt{\phantom{x}}$  and  $\log$  will reduce the magnitude of large values.
- Powers ( $^2$  and  $^3$ ) will increase the spread in magnitude of large values.

**Important:** You should still understand the *logic* we worked through to determine how best to transform the data. The bulge diagram is just a summary of this same reasoning. You will be expected to be able to explain why a given transformation is or is not appropriate for linearization.

## 8.4.2 Additional Remarks

Visualization requires a lot of thought!

- There are many tools for visualizing distributions.
  - Distribution of a single variable:
    1. Rugplot
    2. Histogram
    3. Density plot
    4. Box plot
    5. Violin plot
  - Joint distribution of two quantitative variables:
    1. Scatter plot
    2. Hex plot
    3. Contour plot

This class primarily uses `seaborn` and `matplotlib`, but `pandas` also has basic built-in plotting methods. Many other visualization libraries exist, and `plotly` is one of them.

- `plotly` creates very easily creates interactive plots.
- `plotly` will occasionally appear in lecture code, labs, and assignments!

Next, we'll go deeper into the theory behind visualization.

## 8.5 Visualization Theory

This section marks a pivot to the second major topic of this lecture - visualization theory. We'll discuss the abstract nature of visualizations and analyze how they convey information.

Remember, we had two goals for visualizing data. This section is particularly important in:

1. Helping us understand the data and results,
2. Communicating our results and conclusions with others.

### 8.5.1 Information Channels

Visualizations are able to convey information through various encodings. In the remainder of this lecture, we'll look at the use of color, scale, and depth, to name a few.

#### 8.5.1.1 Encodings in Rugplots

One detail that we may have overlooked in our earlier discussion of rugplots is the importance of encodings. Rugplots are effective visuals because they utilize line thickness to encode frequency. Consider the following diagram:

#### 8.5.1.2 Multi-Dimensional Encodings

Encodings are also useful for representing multi-dimensional data. Notice how the following visual highlights four distinct “dimensions” of data:

- X-axis
- Y-axis
- Area
- Color

The human visual perception system is only capable of visualizing data in a three-dimensional plane, but as you've seen, we can encode many more channels of information.

## 8.5.2 Harnessing X|Y

### 8.5.2.1 Consider the Scale of the Data

However, we should be careful to not misrepresent relationships in our data by manipulating the scale or axes. The visualization below improperly portrays two seemingly independent relationships on the same plot. The authors have clearly changed the scale of the y-axis to mislead their audience.

Notice how the downwards-facing line segment contains values in the millions, while the upwards-trending segment only contains values near three hundred thousand. These lines should not be intersecting.

When there is a large difference in the magnitude of the data, it's advised to analyze percentages instead of counts. The following diagrams correctly display the trends in cancer screening and abortion rates.

### 8.5.2.2 Reveal the Data

Great visualizations not only consider the scale of the data but also utilize the axes in a way that best conveys information. For example, data scientists commonly set certain axes limits to highlight parts of the visualization they are most interested in.

The visualization on the right captures the trend in coronavirus cases during March of 2020. From only looking at the visualization on the left, a viewer may incorrectly believe that coronavirus began to skyrocket on March 4<sup>th</sup>, 2020. However, the second illustration tells a different story - cases rose closer to March 21<sup>th</sup>, 2020.

## 8.5.3 Harnessing Color

Color is another important feature in visualizations that does more than what meets the eye.

We already explored using color to encode a categorical variable in our scatter plot. Let's now discuss the uses of color in novel visualizations like colormaps and heatmaps.

5-8% of the world is red-green color blind, so we have to be very particular about our color scheme. We want to make these as accessible as possible. Choosing a set of colors that work together is evidently a challenging task!



### 8.5.3.1 Colormaps

Colormaps are mappings from pixel data to color values, and they're often used to highlight distinct parts of an image. Let's investigate a few properties of colormaps.

#### Jet Colormap

#### Viridis Colormap

The jet colormap is infamous for being misleading. While it seems more vibrant than viridis, the aggressive colors poorly encode numerical data. To understand why, let's analyze the following images.

The diagram on the left compares how a variety of colormaps represent pixel data that transitions from a high to low intensity. These include the jet colormap (row a) and grayscale (row b). Notice how the grayscale images do the best job in smoothly transitioning between pixel data. The jet colormap is the worst at this - the four images in row (a) look like a conglomeration of individual colors.

The difference is also evident in the images labeled (a) and (b) on the left side. The grayscale image is better at preserving finer detail in the vertical line strokes. Additionally, grayscale is preferred in X-ray scans for being more neutral. The intensity of the dark red color in the jet colormap is frightening and indicates something is wrong.

Why is the jet colormap so much worse? The answer lies in how its color composition is perceived to the human eye.

#### Jet Colormap Perception

#### Viridis Colormap Perception

The jet colormap is largely misleading because it is not perceptually uniform. **Perceptually uniform colormaps** have the property that if the pixel data goes from 0.1 to 0.2, the perceptual change is the same as when the data goes from 0.8 to 0.9.

Notice how the said uniformity is present within the linear trend displayed in the viridis colormap. On the other hand, the jet colormap is largely non-linear - this is precisely why it's considered a worse colormap.

### 8.5.4 Harnessing Markings

In our earlier discussion of multi-dimensional encodings, we analyzed a scatter plot with four pseudo-dimensions: the two axes, area, and color. Were these appropriate to use? The following diagram analyzes how well the human eye can distinguish between these "markings".

There are a few key takeaways from this diagram

- Lengths are easy to discern. Don't use plots with jiggled baselines - keep everything axis-aligned.
- Avoid pie charts! Angle judgments are inaccurate.
- Areas and volumes are hard to distinguish (area charts, word clouds, etc.).

### 8.5.5 Harnessing Conditioning

Conditioning is the process of comparing data that belong to separate groups. We've seen this before in overlaid distributions, side-by-side box plots, and scatter plots with categorical encodings. Here, we'll introduce terminology that formalizes these examples.

Consider an example where we want to analyze income earnings for males and females with varying levels of education. There are multiple ways to compare this data.

The barplot is an example of **juxtaposition**: placing multiple plots side by side, with the same scale. The scatter plot is an example of **superposition**: placing multiple density curves and scatter plots on top of each other.

Which is better depends on the problem at hand. Here, superposition makes the precise wage difference very clear from a quick glance. However, many sophisticated plots convey information that favors the use of juxtaposition. Below is one example.

### 8.5.6 Harnessing Context

The last component of a great visualization is perhaps the most critical - the use of context. Adding informative titles, axis labels, and descriptive captions are all best practices that we've heard repeatedly in Data 8.

A publication-ready plot (and every Data 100 plot) needs:

- **Informative title (takeaway, not description),**
- **Axis labels,**
- Reference lines, markers, etc,
- Legends, if appropriate,
- Captions that describe data,

Captions should:

- Be comprehensive and self-contained,
- Describe what has been graphed,
- Draw attention to important features,
- Describe conclusions drawn from graphs.

## 9 Sampling

### **i** Learning Outcomes

- Understand how to appropriately collect data to help answer a question.

In data science, understanding characteristics of a population starts with having quality data to investigate. While it is often impossible to collect all the data describing a population, we can overcome this by properly sampling from the population. In this note, we will discuss appropriate techniques for sampling from populations.

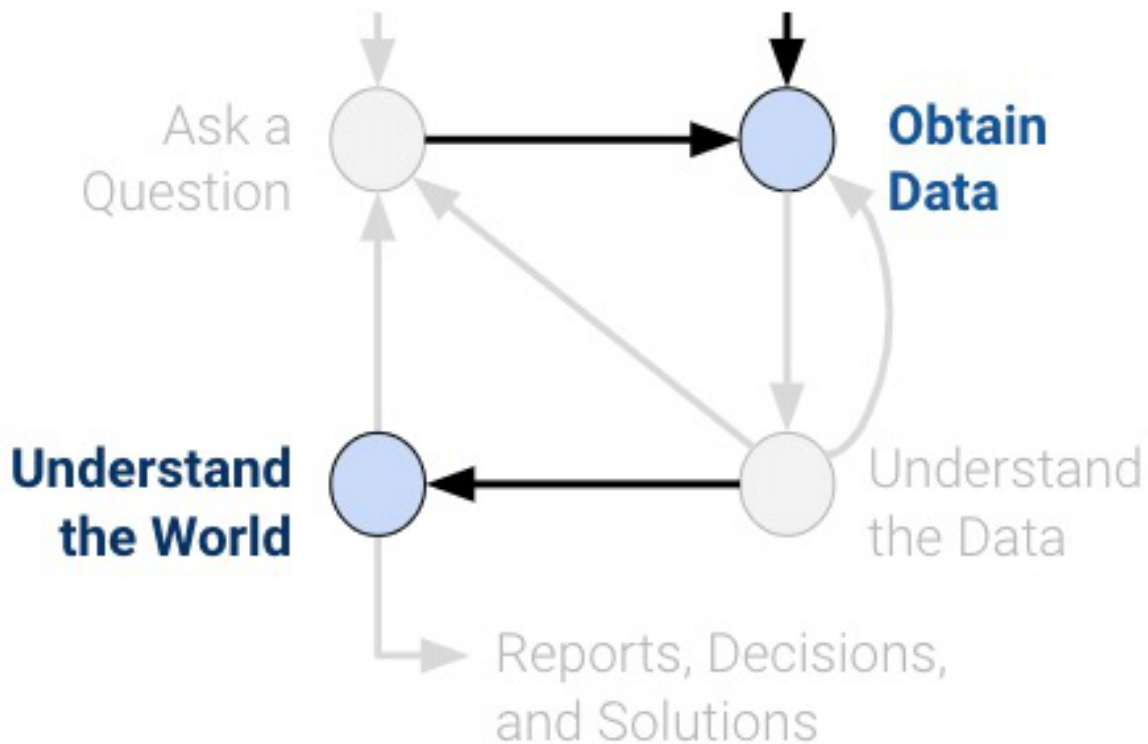


Figure 9.1: Lifecycle diagram

## 9.1 Censuses and Surveys

In general: a **census** is “a complete count or survey of a **population**, typically recording various details of **individuals**.” An example is the U.S. Decennial Census which was held in April 2020. It counts *every person* living in all 50 states, DC, and US territories, not just citizens. Participation is required by law (it is mandated by the U.S. Constitution). Important uses include the allocation of Federal funds, congressional representation, and drawing congressional and state legislative districts. The census is composed of a **survey** mailed to different housing addresses in the United States.

A **survey** is a set of questions. An example is workers sampling individuals and households. What is asked and how it is asked can affect how the respondent answers or even whether or not they answer in the first place.

While censuses are great, it is often very difficult and expensive to survey everyone in a population. Imagine the amount of resources, money, time, and energy the U.S. spent on the 2020 Census. While this does give us more accurate information about the population, it's often infeasible to execute. Thus, we usually survey a subset of the population instead.

A **sample** is (usually) a subset of the population that is often used to make inferences about the population. If our sample is a good representation of our population, then we can use it to glean useful information at a lower cost. That being said, how the sample is drawn will affect the reliability of such inferences. Two common sources of error in sampling are **chance error**, where random samples can vary from what is expected in any direction, and **bias**, which is a systematic error in one direction. Biases can be the result of many things, for example, our sampling scheme or survey methods.

Let's define some useful vocabulary:

- **Population:** The group that you want to learn something about.
  - **Individuals** in a population are not always people. Other populations include bacteria in your gut (sampled using DNA sequencing), trees of a certain species, small businesses receiving a microloan, or published results in an academic journal or field.
- **Sampling Frame:** The list from which the sample is drawn.
  - For example, if sampling people, then the sampling frame is the set of all people that could possibly end up in your sample.
- **Sample:** Who you actually end up sampling. The sample is therefore a subset of your *sampling frame*.

While ideally, these three sets would be exactly the same, they usually aren't in practice. For example, there may be individuals in your sampling frame (and hence, your sample) that are not in your population. And generally, sample sizes are much smaller than population sizes.

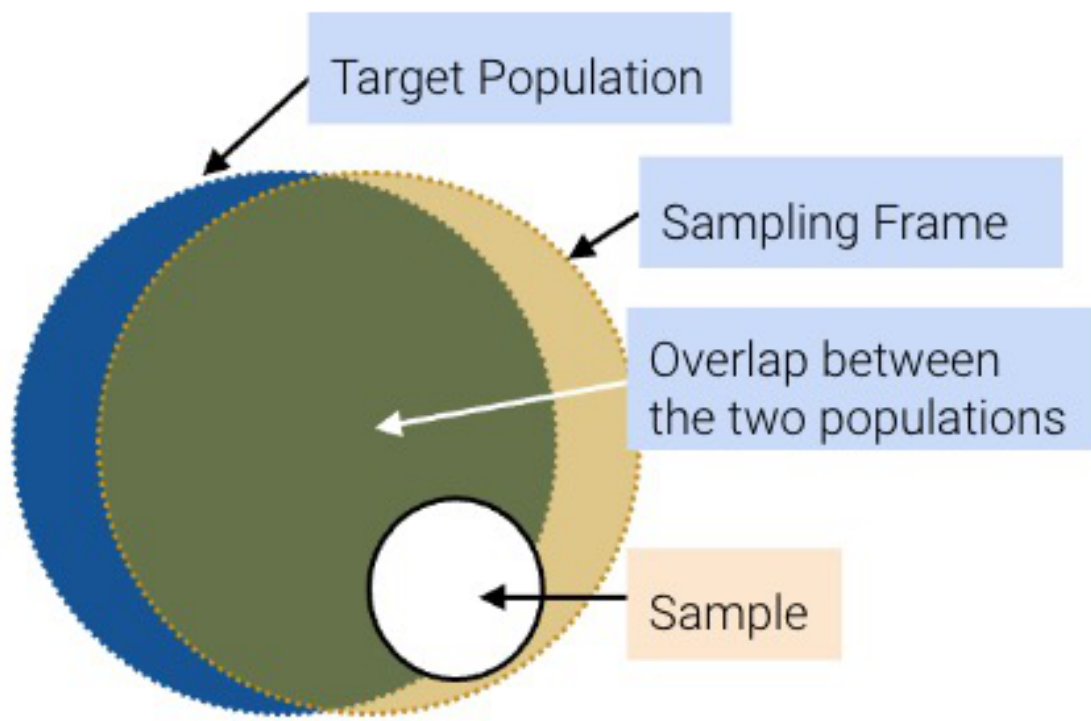


Figure 9.2: Sampling\_Frames

## 9.2 Sampling: A Case Study

The following case study is adapted from *Statistics* by Freedman, Pisani, and Purves, W.W. Norton NY, 1978.

In 1936, President Franklin D. Roosevelt (Democratic) went up for re-election against Alf Landon (Republican). As is usual, **polls** were conducted in the months leading up to the election to try and predict the outcome. The *Literary Digest* was a magazine that had successfully predicted the outcome of 5 general elections coming into 1936. In their polling for the 1936 election, they sent out their survey to 10 million individuals whom they found from phone books, lists of magazine subscribers, and lists of country club members. Of the roughly 2.4 million people who filled out the survey, only 43% reported they would vote for Roosevelt; thus, the *Digest* predicted that Landon would win.

On election day, Roosevelt won in a landslide, winning 61% of the popular vote of about 45 million voters. How could the *Digest* have been so wrong with their polling?

It turns out that the *Literary Digest* sample was not representative of the population. Their sampling frame of people found in phone books, lists of magazine subscribers, and lists of

country club members were more affluent and tended to vote Republican. As such, their sampling frame was inherently skewed in Landon's favor. The *Literary Digest* completely overlooked the lion's share of voters who were still suffering through the Great Depression. Furthermore, they had a dismal response rate (about 24%); who knows how the other non-respondents would have polled? The *Digest* folded just 18 months after this disaster.

At the same time, George Gallup, a rising statistician, also made predictions about the 1936 elections. Despite having a smaller sample size of "only" 50,000 (this is still more than necessary; more when we cover the Central Limit Theorem), his estimate that 56% of voters would choose Roosevelt was much closer to the actual result (61%). Gallup also predicted the *Digest's* prediction within 1% with a sample size of only 3000 people by anticipating the *Digest's* affluent sampling frame and subsampling those individuals.

## 9.3 Sampling Errors

So what's the moral of the story? Samples, while convenient, are subject to chance error and **bias**. Election polling, in particular, can involve many sources of bias. To name a few:

- **Selection bias** systematically excludes (or favors) particular groups.
  - Example: the Literary Digest poll excludes people not in phone books.
  - How to avoid: Randomly sample, and improve overlap of sampling frame and population.
- **Response bias** occurs because people don't always respond truthfully. Survey designers pay special detail to the nature and wording of questions to avoid this type of bias.
  - Example: Illegal immigrants might not answer truthfully when asked citizenship questions on the census survey.
  - How to avoid: Improve questions. Lots of response bias [subtypes + prevention methods](#).
- **Non-response bias** occurs because people don't always respond to survey requests, which can skew responses.
  - Example: Only 2.4m out of 10m people responded to the *Literary Digest's* poll.
  - How to avoid: Increase response rate. For example, reduce the number and length of questions, incentivize completion, and follow up.

## 9.4 Types of Sampling

When sampling, it is essential to focus on the quality of the sample rather than the quantity of the sample. A huge sample size does not fix a bad sampling method. Our main goal is to

gather a sample that is representative of the population it came from. In this section, we'll explore the different types of sampling and their pros and cons.

A **convenience sample** is whatever you can get ahold of; this type of sampling is *non-random*. Note that haphazard sampling is not necessarily random sampling; there are many potential sources of bias.

In a **probability sample**, we provide the **chance** that any specified **set** of individuals will be in the sample (individuals in the population can have different chances of being selected; they don't all have to be uniform), and we sample at random based off this known chance. For this reason, probability samples are also called **random samples**. The randomness provides a few benefits:

- Because we know the source probabilities, we can **measure the errors**.
- Sampling at random gives us a more representative sample of the population, which **reduces bias**. (Note: this is only the case when the probability distribution we're sampling from is accurate. Random samples using "bad" or inaccurate distributions can produce biased estimates of population quantities.)
- Probability samples allow us to **estimate** the **bias** and **chance error**, which helps us **quantify uncertainty** (more in a future lecture).

The real world is usually more complicated, and we often don't know the initial probabilities. For example, we do not generally know the probability that a given bacterium is in a microbiome sample or whether people will answer when Gallup calls landlines. That being said, still we try to model probability sampling to the best of our ability even when the sampling or measurement process is not fully under our control.

A few common random sampling schemes:

- A **uniform random sample with replacement** is a sample drawn **uniformly** at random **with** replacement.
  - Random doesn't always mean "uniformly at random," but in this specific context, it does.
  - Some individuals in the population might get picked more than once.
- A **simple random sample (SRS)** is a sample drawn **uniformly** at random **without** replacement.
  - Every individual (and subset of individuals) has the same chance of being selected from the sampling frame.
  - Every pair has the same chance as every other pair.
  - Every triple has the same chance as every other triple.
  - And so on.
- A **stratified random sample**, where random sampling is performed on strata (specific groups), and the groups together compose a sample.

### 9.4.1 Example Scheme 1: Probability Sample

Suppose we have 3 TA's (Arman, Boyu, Charlie): I decide to sample 2 of them as follows:

- I choose A with probability 1.0
- I choose either B or C, each with a probability of 0.5.

We can list all the possible outcomes and their respective probabilities in a table:

Outcome	Probability
{A, B}	0.5
{A, C}	0.5
{B, C}	0

This is a **probability sample** (though not a great one). Of the 3 people in my population, I know the chance of getting each subset. Suppose I'm measuring the average distance TAs live from campus.

- This scheme does not see the entire population!
- My estimate using the single sample I take has some chance error depending on if I see AB or AC.
- This scheme is biased towards A's response.

### 9.4.2 Example Scheme 2: Simple Random Sample

Consider the following sampling scheme:

- A class roster has 1100 students listed alphabetically.
- Pick one of the first 10 students on the list at random (e.g. Student 8).
- To create your sample, take that student and every 10th student listed after that (e.g. Students 8, 18, 28, 38, etc.).

Is this a probability sample?

Yes. For a sample  $[n, n + 10, n + 20, \dots, n + 1090]$ , where  $1 \leq n \leq 10$ , the probability of that sample is  $1/10$ . Otherwise, the probability is 0.

Only 10 possible samples!

Does each student have the same probability of being selected?

Yes. Each student is chosen with a probability of  $1/10$ .

Is this a simple random sample?

No. The chance of selecting (8, 18) is  $1/10$ ; the chance of selecting (8, 9) is 0.



### 9.4.3 Example Scheme 3: Stratified Random Sampling

Suppose you want to interview a representative sample of **12 students** enrolled in Data 100.

- Suppose there are **1,200 students** in Data 100.
- **100 students** are graduate students. The remaining **1,100** are undergraduates.
- I conduct an SRS with **n=1** on the 100 graduate students, and an SRS with **n=11** on the 1,100 undergraduates.

Does each student have the same probability of being selected?

**Yes.** Each student is chosen with probability 1/100

Is there any benefit or downside to sampling this way?

**Yes, a benefit!** We have **guaranteed proportional representation** of undergrads and grad students. In other words, we have **reduced chance error** (i.e., variance).

## 9.5 Demo: The 1936 Presidential Election Results

Let's start with the real election results from the 1936 election.

- Each row of `votes` represents a single voter.
- `voted_dem` is 0/1 variable indicating whether the voter voted for Franklin D. Roosevelt, who was the Democratic candidate in 1936. If 0, the voter voted for Alf Landon, the Republican candidate.

Votes for other parties are excluded from this dataset.

```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
import zipfile

sns.set_theme(style='darkgrid', font_scale = 1.5,
               rc={'figure.figsize':(7,5)})
```

```
with zipfile.ZipFile("data/1936_votes.zip", 'r') as z:
    with z.open("1936_votes.csv") as csv_file:
        votes = pd.read_csv(csv_file)

votes.head()
```

	voted_dem
0	1
1	1
2	0
3	1
4	1

How many votes were cast for either Roosevelt or Landon in 1936?

```
len(votes)
```

44430549

What fraction of voters voted for Roosevelt, the Democratic candidate?

```
votes['voted_dem'].sum() / len(votes)
```

np.float64(0.6245897614274358)

But wait, don't the slides say that Roosevelt won 61% of the vote?

Yes! But, he won 61% of **all** votes. If we filter to just the voters who voted for Roosevelt or Landon, Roosevelt won 62.5% of votes.

Useful tip: The mean of a 0/1 column is the same as the proportion of values that are 1.

```
votes['voted_dem'].mean()
```

np.float64(0.6245897614274358)

Of the **44,430,549** voters who voted for either Roosevelt or Landon, **62.5%** voted for Roosevelt.

### 9.5.1 Simple Random Sample (SRS)

Note: An SRS is sometimes called a “names in a hat” sample, since it’s a lot like putting each observation on a slip of paper, putting all the slips in a big hat, and then randomly drawing slips one at a time.

If we were to take a simple random sample of just 1,000 voters and calculate the proportion who planned to vote for Roosevelt, how close would we be to 62.5%?

```
votes['voted_dem'].sample(1000).mean()
```

```
np.float64(0.62)
```

Note that the cell above is a little slow, since we’re sampling from a `DataFrame` with almost 45 million rows.

We can speed up the sampling using NumPy:

```
# Construct a random number generator object.
# No need to be familiar with using NumPy this way in Data 100!
rng = np.random.default_rng()

n_votes = len(votes)

# Generate 1000 random integers from 0 to (number of votes - 1)
idx = rng.integers(low=0, high=n_votes-1, size=1000)

votes['voted_dem'].iloc[idx].mean()
```

```
np.float64(0.593)
```

Both of the estimates above are pretty close to 62.5%! They are much closer than the estimate from the Literary Digest poll, which predicted that 43% of votes would go to Roosevelt.

This is no fluke! If we repeat this over and over, we tend to hover around 62.5%.

```
for _ in range(10):
    idx = rng.integers(low=0, high=n_votes-1, size=1000)
    print(votes['voted_dem'].iloc[idx].mean())
```

```
0.622
0.66
0.63
0.599
0.607
0.616
0.608
0.625
0.627
0.601
```

Let's randomly generate 10,000 estimates:

```
nrep = 10000    # number of simulations
n = 1000        # size of our sample
results = []    # list to store the sampling results

for i in range(0, nrep):
    idx = rng.integers(low=0, high=n_votes, size=1000)
    results.append(votes['voted_dem'].iloc[idx].mean())

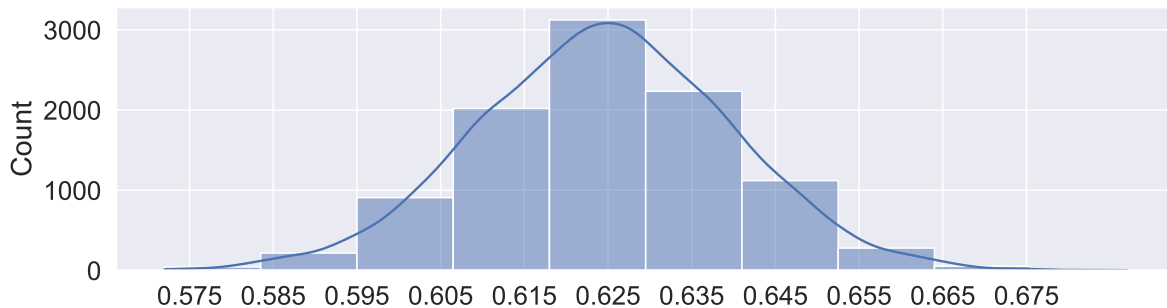
# First 10 simulated sample proportions
results[:10]
```

```
[np.float64(0.617),
 np.float64(0.623),
 np.float64(0.617),
 np.float64(0.608),
 np.float64(0.628),
 np.float64(0.629),
 np.float64(0.631),
 np.float64(0.622),
 np.float64(0.629),
 np.float64(0.623)]
```

Plotting our estimates with KDE:

```
plt.figure(figsize=(12, 3))
p = sns.histplot(x=results, kde=True, bins=10)

# Make x-axis centered at 0.625 with 0.01 intervals
p.set_xticks(np.arange(0.625 - 5 * 0.01, 0.625 + 5 * 0.01, 0.01));
```



We get an approximate normal distribution centered around 62.5%, with most of the mass of the distribution (say, 95% of the mass) within about 3 percentage points (0.03) on each side.

As it turns out, with a sample size of 1000, our estimate of the proportion of voters supporting Roosevelt has a margin of error of about 3 percentage points (3pp) at a 95% confidence level (CL), so long as we take a simple random sample (SRS) of actual voters.

- Note: You tend to see 3pp and 95% CL quite a lot in political polling!

We'll learn what these values mean and how to calculate them when we (re)learn the Central Limit Theorem later in the semester.

## 9.6 Demo: Revisiting the 1936 Literary Digest Poll

The `poll` DataFrame contains a summary of the 1936 Literary Digest Poll, along with polling results and actual election results from 1932 and 1936.

- Each row of `poll` represents a U.S. state.
- `state`: name of the U.S. state.
- `electoral_votes`: # electoral votes allocated to the given state.
- `actual_dem_1936`: # votes for Roosevelt (the Democratic candidate) in 1936.
- `actual_rep_1936`: # votes for Landon (the Republican candidate) in 1936.
- `ld_dem_1936`: # Literary Digest respondents who planned to vote for Roosevelt in 1936.
- `ld_rep_1936`: # Literary Digest respondents who planned to vote for Landon in 1936.

Literary Digest also had a 1932 poll! We will use this data for post-stratification: \* `actual_dem_1932`: # votes for the Democratic candidate in 1932. \* `actual_rep_1932`: # votes for the Republican candidate in 1932. \* `ld_dem_1932`: # of 1936 Literary Digest respondents who voted for the Democratic candidate in 1932. \* `ld_rep_1932`: # of 1936 Literary Digest respondents who voted for Republican candidate in 1932.

Note: Votes from parties other than Democratic and Republican are excluded from this dataset.

```
poll = pd.read_csv('data/literary-digest-summary-data.csv')
poll.head()
```

	state	electoral_votes	actual_dem_1936	actual_rep_1936	ld_rep_1936	ld_dem_1936	actual_dem_1936
0	Alabama	11	238196	35358	3060	10082	2079
1	Arizona	3	86722	33433	2337	1975	7926
2	Arkansas	9	146765	32049	2724	7608	1896
3	California	22	1766836	836431	89516	77245	1324
4	Colorado	6	295021	181267	15949	10025	2508

As a sanity check, let's make sure we have the same number of votes as the first dataset (44,430,549):

```
poll['actual_dem_1936'].sum() + poll['actual_rep_1936'].sum()
```

```
np.int64(44430549)
```

Let's also check that we get the reported Literary Digest prediction of 43% for Roosevelt.

- Remember, Roosevelt received 62.5% of the actual vote.

```
poll['ld_dem_1936'].sum() / (poll['ld_dem_1936'].sum() + poll['ld_rep_1936'].sum())
```

```
np.float64(0.4289439704056572)
```

### 9.6.1 Post-stratification with Literary Digest responses from 1932 and 1936

Using **post-stratification**, let's see if we can improve the Literary Digest poll result using the **same information available to Literary Digest in 1936**.

- In other words, without using data from the future!

Recall the steps of post-stratification:

1. Divide the sample and population into cells defined by chosen characteristics.
2. Calculate the overall response in each sample cell.
3. Aggregate over sample cells, reweighting by the size of the corresponding population cell.

**Sample:** Responses to the Literary Digest poll from 1932, among 1936 poll respondents

**Population:** The actual election outcomes in 1932

**Cells:** Every combination of state and political party

Wait, aren't we interested in the 1936 Literary Digest poll?

- Yes! But, we can use responses from the older 1932 poll and 1932 election results to get our **sample cell weights**, and then use these weights to turn the 1936 poll results into a prediction of the 1936 election results.
- Note that this approach assumes that over- and under-representation of voters among the poll respondents in state and party is the same in 1932 and 1936!

Let's start with step 1. We divide our population and sample into cells defined by each combination of **state** and **choice of party in 1932**:

- Cell 1: Alabama + Republican in 1932
- Cell 2: Alabama + Democratic in 1932
- Cell 3: Arizona + Republican in 1932
- Cell 4: Arizona + Democratic in 1932
- ...

Note: Alaska and Hawaii were not U.S. states until after 1936.

The population cells are already in `polls`: `actual_dem_1932` and `actual_rep_1932` provide the actual vote counts for each party and state in 1932.

The sample cells are also in `polls`: `ld_dem_1932` and `ld_rep_1932` provide the number of responses to the 1932 Literary Digest poll, among 1936 poll respondents, for each party.

Let's make the **big** assumption that respondents in `ld_dem_1932` are representative of all voters in `actual_dem_1932` for each state, and the same for `ld_rep_1932` and `actual_rep_1932`.

- In other words, we claim that response rates and outreach for Democrats and Republicans from each state in 1932 can differ, but ultimately **poll respondents from a particular party+state combination are representative of actual voters for each party+state combination**.
- Then, we can calculate the **reweighting factor**, or how over- or under-represented poll respondents are relative to actual voters.
- All we need to do is divide the actual vote counts by the corresponding number of respondents, for each combination of party and state.

```
poll['dem_reweight_factor'] = poll['actual_dem_1932'] / poll['ld_dem_1932']
poll['rep_reweight_factor'] = poll['actual_rep_1932'] / poll['ld_rep_1932']
poll.tail()
```

	state	electoral_votes	actual_dem_1936	actual_rep_1936	ld_rep_1936	ld_dem_1936	actual_dem_1936
43	Virginia	11	234980	98336	10223	16783	
44	Washington	8	459579	206892	21370	15300	
45	West Virginia	8	502582	325358	13660	10235	
46	Wisconsin	12	802984	380828	33796	20781	
47	Wyoming	3	62624	38739	2526	1533	

Note that `dem_reweight_factor` is about 36 for Arizona.

- In other words, there were 36 times as many Democratic voters in Arizona than Democratic poll respondents.

Similarly, `rep_reweight_factor` is about 21.5 for Arizona.

- So, Democratic voters are **underrepresented** in the 1932 Literary Digest poll responses, relative to Republican voters.
- Based on the Republican bias in the Literary Digest sample discussed in lecture (i.e., wealthier folks with phones, cars, and magazines), this is expected!

Next, we apply these same weights to inflate the 1936 poll results into vote predictions.

- Again, note that this approach assumes over- and under-representation patterns are the same in the 1932 and 1936 polls!

```
poll['pred_dem_1936'] = round(poll['ld_dem_1936'] * poll['dem_reweight_factor'])
poll['pred_rep_1936'] = round(poll['ld_rep_1936'] * poll['rep_reweight_factor'])
poll.head()
```

	state	electoral_votes	actual_dem_1936	actual_rep_1936	ld_rep_1936	ld_dem_1936	actual_dem_1936
0	Alabama	11	238196	35358	3060	10082	2079
1	Arizona	3	86722	33433	2337	1975	7926
2	Arkansas	9	146765	32049	2724	7608	1896
3	California	22	1766836	836431	89516	77245	1324
4	Colorado	6	295021	181267	15949	10025	2508

Finally, let's calculate the proportion of **predicted** votes that are allocated to Roosevelt in 1936.



- Remember that Roosevelt received 62.5% of the **actual** vote in 1936.

```
poll['pred_dem_1936'].sum() / (poll['pred_dem_1936'].sum() + poll['pred_rep_1936'].sum())

np.float64(0.5422251022375592)
```

54% is a majority! Using post-stratification, we have shifted the Literary Digest prediction of a Roosevelt loss with 43% of the vote to a (correct) Roosevelt win with 54%.

- There is no cheating here; we used the same data available to Literary Digest in 1936.
- Note that post-stratification is not perfect. We are still off by almost 10 percentage points. But, we've moved in the right direction.

## 9.7 Bonus: Follow Up Improvements

As a follow-up exercise, we can compare the predicted 1936 vote totals to the actual 1932 vote totals.

- Then, we could apply a **correction factor** to change the predicted number of 1936 votes to be in line with the total number of votes in 1932.
- This exercise assumes that the total number of votes cast in 1932 would be the same in 1936, but the poll response rates and outreach might change between 1932 and 1936.

```
poll['pred_total_1936'] = poll['pred_dem_1936'] + poll['pred_rep_1936']
poll['actual_total_1932'] = poll['actual_dem_1932'] + poll['actual_rep_1932']
poll['correction_factor'] = poll['actual_total_1932'] / poll['pred_total_1936']
poll.head()
```

	state	electoral_votes	actual_dem_1936	actual_rep_1936	ld_rep_1936	ld_dem_1936	actual_dem_1932
0	Alabama	11	238196	35358	3060	10082	2079
1	Arizona	3	86722	33433	2337	1975	7926
2	Arkansas	9	146765	32049	2724	7608	1896
3	California	22	1766836	836431	89516	77245	1324
4	Colorado	6	295021	181267	15949	10025	2508

```
poll['pred_dem_1936_corrected'] = poll['pred_dem_1936'] * poll['correction_factor']
poll['pred_rep_1936_corrected'] = poll['pred_rep_1936'] * poll['correction_factor']

poll['pred_dem_1936_corrected'].sum() / (poll['pred_dem_1936_corrected'].sum() + poll['pred_rep_1936_corrected'].sum())
```

```
np.float64(0.5419440974611633)
```

Looks like a pretty similar prediction for Roosevelt of 54%.

As it turns out, it looks like our original (i.e., uncorrected) predictions had a vote total closer to the true 1936 vote total:

```
print('Actual 1936 vote total:')
print(poll['actual_dem_1936'].sum() + poll['actual_rep_1936'].sum())

print('Predicted 1936 vote total, uncorrected:')
print(poll['pred_dem_1936'].sum() + poll['pred_rep_1936'].sum())

print('Predicted 1936 vote total, corrected:')
print(poll['pred_dem_1936_corrected'].sum() + poll['pred_rep_1936_corrected'].sum())
```

```
Actual 1936 vote total:
44430549
Predicted 1936 vote total, uncorrected:
42058418.0
Predicted 1936 vote total, corrected:
38582531.0
```

Furthermore, we can check whether post-stratification would have led to a predicted win for Roosevelt in the electoral college, which is what actually determines the election outcome.

- To do this, we allocate **all** of the electoral votes in each state to the candidate with the most predicted votes in that state, and then sum up the total number of electoral votes allocated to each candidate across states.

```
poll['dem_wins'] = poll['pred_dem_1936'] > poll['pred_rep_1936']

print('Total predicted Roosevelt electoral votes:')
print(( poll['dem_wins'] * poll['electoral_votes'] ).sum())

print('Total predicted Landon electoral votes:')
print(( (1-poll['dem_wins']) * poll['electoral_votes'] ).sum())
```

```
Total predicted Roosevelt electoral votes:
380
Total predicted Landon electoral votes:
151
```

We (correctly) predict a Roosevelt landslide in the electoral college!

- But, note that the actual electoral college landslide was much bigger: 523 to 8
- This is the largest electoral college landslide since 1820 (as of 2025).

## 9.8 Summary

Understanding the sampling process is what lets us go from describing the data to understanding the world. Without knowing / assuming something about how the data were collected, there is no connection between the sample and the population. Ultimately, the dataset doesn't tell us about the world behind the data.

# 10 Modeling & SLR

## Learning Outcomes

- Understand what models are and how to carry out the four-step modeling process.
- Define the concept of loss and gain familiarity with  $L_1$  and  $L_2$  loss.
- Fit the Simple Linear Regression model using minimization techniques.

Up until this point in the semester, we've focused on analyzing datasets. We've looked into the early stages of the data science lifecycle, focusing on the programming tools, visualization techniques, and data cleaning methods needed for data analysis.

This lecture marks a shift in focus. We will move away from examining datasets to actually *using* our data to better understand the world. Specifically, the next sequence of lectures will explore predictive modeling: generating models to make some predictions about the world around us. In this lecture, we'll introduce the conceptual framework for setting up a modeling task. In the next few lectures, we'll put this framework into practice by implementing various kinds of models.

## 10.1 What is a Model?

A model is an **idealized representation** of a system. A system is a set of principles or procedures according to which something functions. We live in a world full of systems: the procedure of turning on a light happens according to a specific set of rules dictating the flow of electricity. The truth behind how any event occurs is usually complex, and many times the specifics are unknown. The workings of the world can be viewed as its own giant procedure. Models seek to simplify the world and distill them into workable pieces.

Example: We model the fall of an object on Earth as subject to a constant acceleration of  $9.81m/s^2$  due to gravity.

- While this describes the behavior of our system, it is merely an approximation.
- It doesn't account for the effects of air resistance, local variations in gravity, etc.
- In practice, it's accurate enough to be useful!

### 10.1.1 Reasons for Building Models

Why do we want to build models? As far as data scientists and statisticians are concerned, there are three reasons, and each implies a different focus on modeling.

1. To explain complex phenomena occurring in the world we live in. Examples of this might be:
  - How are the parents' average height related to their children's average height?
  - How does an object's velocity and acceleration impact how far it travels? (Physics:  $d = d_0 + vt + \frac{1}{2}at^2$ )

In these cases, we care about creating models that are *simple and interpretable*, allowing us to understand what the relationships between our variables are.

2. To make accurate predictions about unseen data. Some examples include:
  - Can we predict if an email is spam or not?
  - Can we generate a one-sentence summary of this 10-page long article?

When making predictions, we care more about making extremely accurate predictions, at the cost of having an uninterpretable model. These are sometimes called black-box models and are common in fields like deep learning.

3. To measure the causal effects of one event on some other event. For example,
  - Does smoking *cause* lung cancer?
  - Does a job training program *cause* increases in employment and wages?

This is a much harder question because most statistical tools are designed to infer association, not causation. We will not focus on this task in Data 100, but you can take other advanced classes on causal inference (e.g., Stat 156, Data 102) if you are intrigued!

Most of the time, we aim to strike a balance between building **interpretable** models and building **accurate models**.

### 10.1.2 Common Types of Models

In general, models can be split into two categories:

1. Deterministic physical (mechanistic) models: Laws that govern how the world works.
  - [Kepler's Third Law of Planetary Motion \(1619\)](#): The ratio of the square of an object's orbital period with the cube of the semi-major axis of its orbit is the same for all objects orbiting the same primary.
    - $T^2 \propto R^3$

- **Newton's Laws: motion and gravitation (1687):** Newton's second law of motion models the relationship between the mass of an object and the force required to accelerate it.
  - $F = ma$
  - $F_g = G \frac{m_1 m_2}{r^2}$
- 2. Probabilistic models: Models that attempt to understand how random processes evolve. These are more general and can be used to describe many phenomena in the real world. These models commonly make simplifying assumptions about the nature of the world.
  - **Poisson Process models:** Used to model random events that happen with some probability at any point in time and are strictly increasing in count, such as the arrival of customers at a store.

Note: These specific models are not in the scope of Data 100 and exist to serve as motivation.

## 10.2 Simple Linear Regression

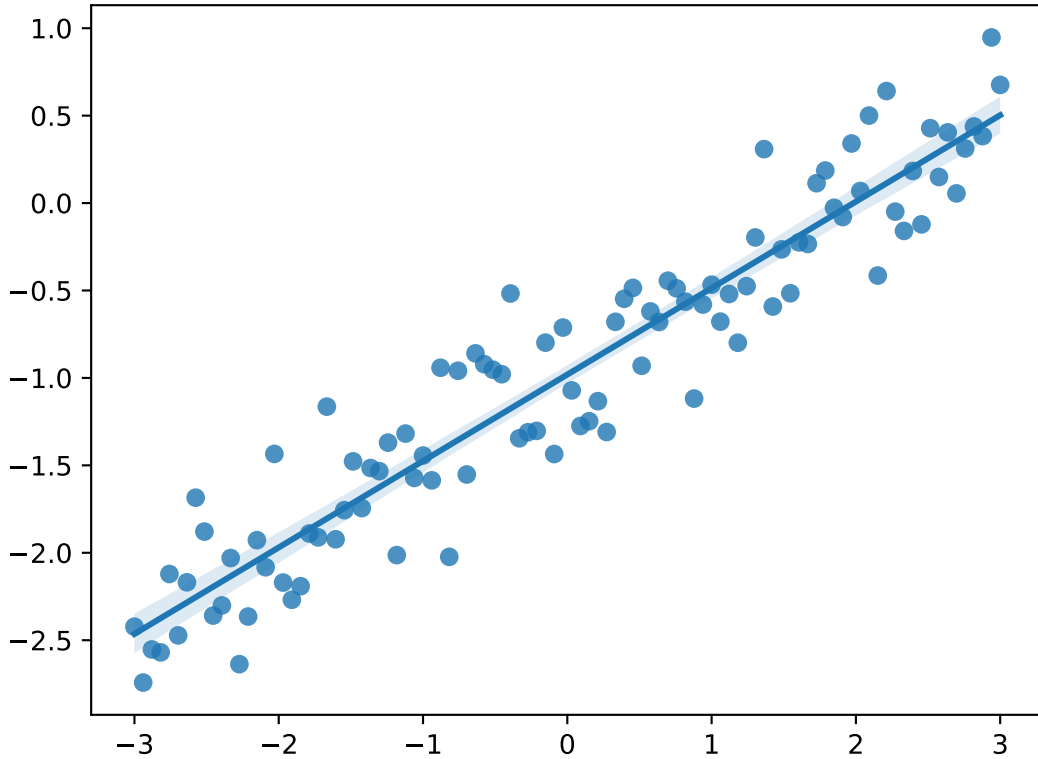
The **regression line** is the unique straight line that minimizes the **mean squared error** of estimation among all straight lines. As with any straight line, it can be defined by a slope and a y-intercept:

- slope =  $r \cdot \frac{\text{Standard Deviation of } y}{\text{Standard Deviation of } x}$
- y-intercept = average of  $y$  – slope · average of  $x$
- regression estimate = y-intercept + slope ·  $x$
- residual = observed  $y$  – regression estimate

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
# Set random seed for consistency
np.random.seed(43)
plt.style.use('default')

# Generate random noise for plotting
x = np.linspace(-3, 3, 100)
y = x * 0.5 - 1 + np.random.randn(100) * 0.3

# Plot regression line
sns.regplot(x=x, y=y);
```



## 10.2.1 Notations and Definitions

For a pair of variables  $x$  and  $y$  representing our data  $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ , we denote their means/averages as  $\bar{x}$  and  $\bar{y}$  and standard deviations as  $\sigma_x$  and  $\sigma_y$ .

### 10.2.1.1 Standard Units

A variable is represented in standard units if the following are true:

1. 0 in standard units is equal to the mean ( $\bar{x}$ ) in the original variable's units.
2. An increase of 1 standard unit is an increase of 1 standard deviation ( $\sigma_x$ ) in the original variable's units.

To convert a variable  $x_i$  into standard units, we subtract its mean from it and divide it by its standard deviation. For example,  $x_i$  in standard units is  $\frac{x_i - \bar{x}}{\sigma_x}$ .

### 10.2.1.2 Correlation

The correlation ( $r$ ) is the average of the product of  $x$  and  $y$ , both measured in *standard units*.

$$r = \frac{1}{n} \sum_{i=1}^n \left( \frac{x_i - \bar{x}}{\sigma_x} \right) \left( \frac{y_i - \bar{y}}{\sigma_y} \right)$$

1. Correlation measures the strength of a **linear association** between two variables.
2. Correlations range between -1 and 1:  $|r| \leq 1$ , with  $r = 1$  indicating perfect positive linear association, and  $r = -1$  indicating perfect negative association. The closer  $r$  is to 0, the weaker the linear association is.
3. Correlation says nothing about causation and non-linear association. Correlation does **not** imply causation. When  $r = 0$ , the two variables are uncorrelated. However, they could still be related through some non-linear relationship.

```
def plot_and_get_corr(ax, x, y, title):
    ax.set_xlim(-3, 3)
    ax.set_ylim(-3, 3)
    ax.set_xticks([])
    ax.set_yticks([])
    ax.scatter(x, y, alpha = 0.73)
    r = np.corrcoef(x, y)[0, 1]
    ax.set_title(title + " (corr: {})".format(r.round(2)))
    return r

fig, axs = plt.subplots(2, 2, figsize = (10, 10))

# Just noise
x1, y1 = np.random.randn(2, 100)
corr1 = plot_and_get_corr(axs[0, 0], x1, y1, title = "noise")

# Strong linear
x2 = np.linspace(-3, 3, 100)
y2 = x2 * 0.5 - 1 + np.random.randn(100) * 0.3
corr2 = plot_and_get_corr(axs[0, 1], x2, y2, title = "strong linear")

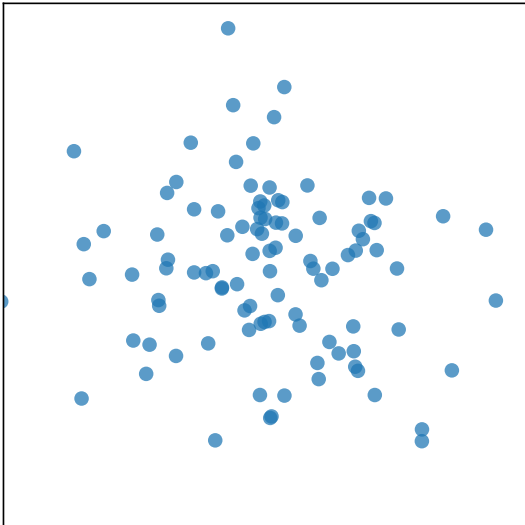
# Unequal spread
x3 = np.linspace(-3, 3, 100)
y3 = - x3/3 + np.random.randn(100)*(x3)/2.5
corr3 = plot_and_get_corr(axs[1, 0], x3, y3, title = "strong linear")
extent = axs[1, 0].get_window_extent().transformed(fig.dpi_scale_trans.inverted())
```



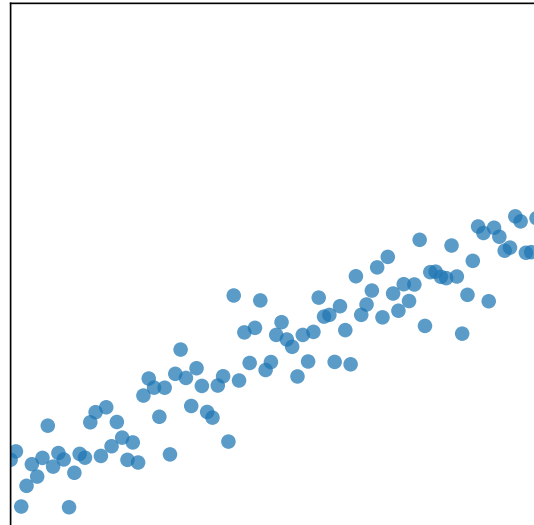
```
# Strong non-linear
x4 = np.linspace(-3, 3, 100)
y4 = 2*np.sin(x3 - 1.5) + np.random.randn(100) * 0.3
corr4 = plot_and_get_corr(axes[1, 1], x4, y4, title = "strong non-linear")

plt.show()
```

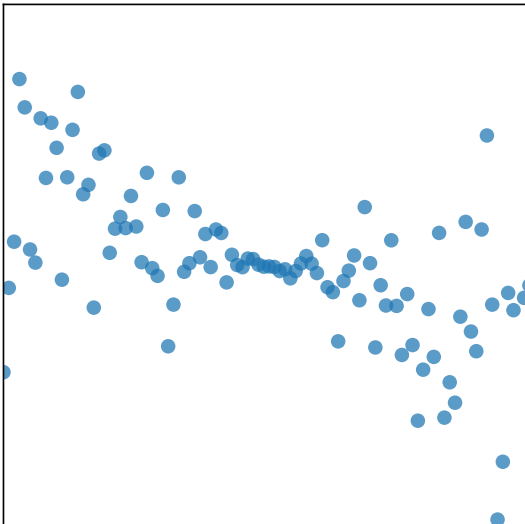
noise (corr: -0.11)



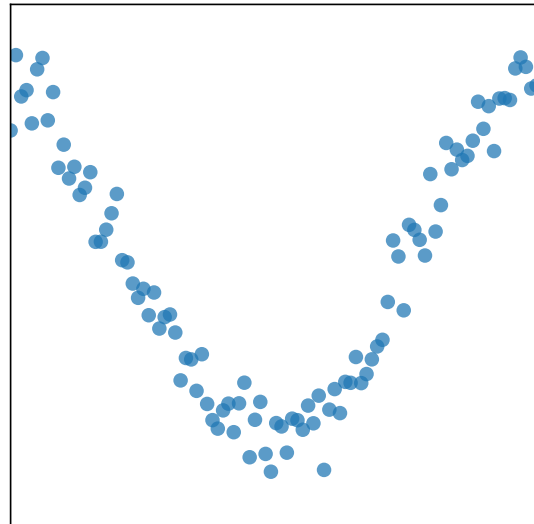
strong linear (corr: 0.94)



strong linear (corr: -0.61)



strong non-linear (corr: 0.06)

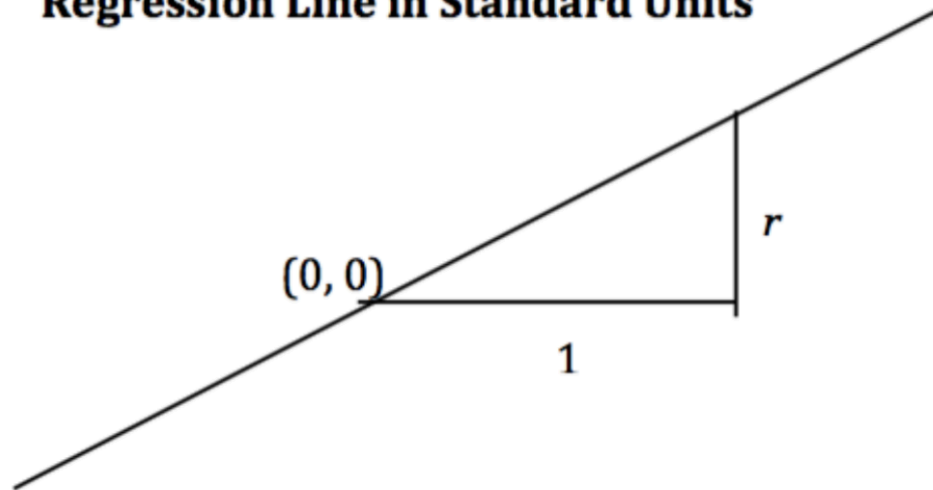


### 10.2.2 Alternate Form

When the variables  $y$  and  $x$  are measured in *standard units*, the regression line for predicting  $y$  based on  $x$  has slope  $r$  and passes through the origin.

$$\hat{y}_{su} = r \cdot x_{su}$$

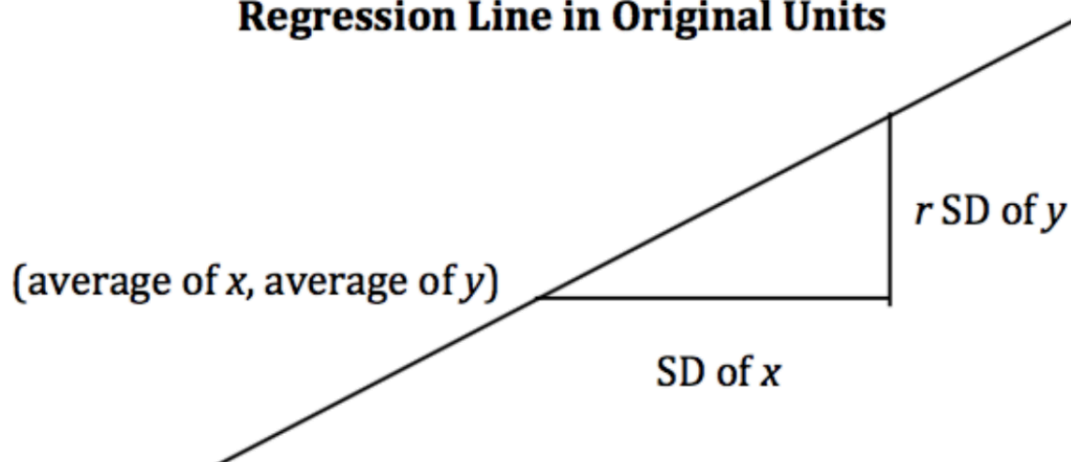
#### Regression Line in Standard Units



- In the original units, this becomes

$$\frac{\hat{y} - \bar{y}}{\sigma_y} = r \cdot \frac{x - \bar{x}}{\sigma_x}$$

## Regression Line in Original Units



### 10.2.3 Derivation

Starting from the top, we have our claimed form of the regression line, and we want to show that it is equivalent to the optimal linear regression line:  $\hat{y} = \hat{a} + \hat{b}x$ .

Recall:

- $\hat{b} = r \cdot \frac{\text{Standard Deviation of } y}{\text{Standard Deviation of } x}$
- $\hat{a} = \text{average of } y - \text{slope} \cdot \text{average of } x$

Proof:

$$\frac{\hat{y} - \bar{y}}{\sigma_y} = r \cdot \frac{x - \bar{x}}{\sigma_x}$$

Multiply by  $\sigma_y$ , and add  $\bar{y}$  on both sides.

$$\hat{y} = \sigma_y \cdot r \cdot \frac{x - \bar{x}}{\sigma_x} + \bar{y}$$

Distribute coefficient  $\sigma_y \cdot r$  to the  $\frac{x - \bar{x}}{\sigma_x}$  term

$$\hat{y} = \left(\frac{r\sigma_y}{\sigma_x}\right) \cdot x + \left(\bar{y} - \left(\frac{r\sigma_y}{\sigma_x}\right)\bar{x}\right)$$

We now see that we have a line that matches our claim:

- slope:  $r \cdot \frac{\text{SD of } y}{\text{SD of } x} = r \cdot \frac{\sigma_y}{\sigma_x}$
- intercept:  $\bar{y} - \text{slope} \cdot \bar{x}$

Note that the error for the i-th datapoint is:  $e_i = y_i - \hat{y}_i$

## 10.3 The Modeling Process

At a high level, a model is a way of representing a system. In Data 100, we'll treat a model as some mathematical rule we use to describe the relationship between variables.

What variables are we modeling? Typically, we use a subset of the variables in our sample of collected data to model another variable in this data. To put this more formally, say we have the following dataset  $\mathcal{D}$ :

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

Each pair of values  $(x_i, y_i)$  represents a datapoint. In a modeling setting, we call these **observations**.  $y_i$  is the dependent variable we are trying to model, also called an **output** or **response**.  $x_i$  is the independent variable inputted into the model to make predictions, also known as a **feature**.

Our goal in modeling is to use the observed data  $\mathcal{D}$  to predict the output variable  $y_i$ . We denote each prediction as  $\hat{y}_i$  (read: “y hat sub i”).

How do we generate these predictions? Some examples of models we'll encounter in the next few lectures are given below:

$$\begin{aligned}\hat{y}_i &= \theta \\ \hat{y}_i &= \theta_0 + \theta_1 x_i\end{aligned}$$

The examples above are known as **parametric models**. They relate the collected data,  $x_i$ , to the prediction we make,  $\hat{y}_i$ . A few parameters ( $\theta, \theta_0, \theta_1$ ) are used to describe the relationship between  $x_i$  and  $\hat{y}_i$ .

Notice that we don't immediately know the values of these parameters. While the features,  $x_i$ , are taken from our observed data, we need to decide what values to give  $\theta, \theta_0$ , and  $\theta_1$  ourselves. This is the heart of parametric modeling: *what parameter values should we choose so our model makes the best possible predictions?*

To choose our model parameters, we'll work through the **modeling process**.

1. Choose a model: how should we represent the world?
2. Choose a loss function: how do we quantify prediction error?
3. Fit the model: how do we choose the best parameters of our model given our data?
4. Evaluate model performance: how do we evaluate whether this process gave rise to a good model?

## 10.4 Choosing a Model

Our first step is choosing a model: defining the mathematical rule that describes the relationship between the features,  $x_i$ , and predictions  $\hat{y}_i$ .

In [Data 8](#), you learned about the **Simple Linear Regression (SLR) model**. You learned that the model takes the form:

$$\hat{y}_i = a + bx_i$$

In [Data 100](#), we'll use slightly different notation: we will replace  $a$  with  $\theta_0$  and  $b$  with  $\theta_1$ . This will allow us to use the same notation when we explore more complex models later on in the course.

$$\hat{y}_i = \theta_0 + \theta_1 x_i$$

The parameters of the SLR model are  $\theta_0$ , also called the intercept term, and  $\theta_1$ , also called the slope term. To create an effective model, we want to choose values for  $\theta_0$  and  $\theta_1$  that most accurately predict the output variable. The “best” fitting model parameters are given the special names:  $\hat{\theta}_0$  and  $\hat{\theta}_1$ ; they are the specific parameter values that allow our model to generate the best possible predictions.

In [Data 8](#), you learned that the best SLR model parameters are:

$$\hat{\theta}_0 = \bar{y} - \hat{\theta}_1 \bar{x} \qquad \hat{\theta}_1 = r \frac{\sigma_y}{\sigma_x}$$

A quick reminder on notation:

- $\bar{y}$  and  $\bar{x}$  indicate the mean value of  $y$  and  $x$ , respectively
- $\sigma_y$  and  $\sigma_x$  indicate the standard deviations of  $y$  and  $x$
- $r$  is the [correlation coefficient](#), defined as the average of the product of  $x$  and  $y$  measured in standard units:  $\frac{1}{n} \sum_{i=1}^n \left( \frac{x_i - \bar{x}}{\sigma_x} \right) \left( \frac{y_i - \bar{y}}{\sigma_y} \right)$

In [Data 100](#), we want to understand *how* to derive these best model coefficients. To do so, we'll introduce the concept of a loss function.

## 10.5 Choosing a Loss Function

We've talked about the idea of creating the “best” possible predictions. This begs the question: how do we decide how “good” or “bad” our model's predictions are?

A **loss function** characterizes the cost, error, or fit resulting from a particular choice of model or model parameters. This function,  $L(y, \hat{y})$ , quantifies how “bad” or “far off” a single prediction by our model is from a true, observed value in our collected data.

The choice of loss function for a particular model will affect the accuracy and computational cost of estimation, and it’ll also depend on the estimation task at hand. For example,

- Are outputs quantitative or qualitative?
- Do outliers matter?
- Are all errors equally costly? (e.g., a false negative on a cancer test is arguably more dangerous than a false positive)

Regardless of the specific function used, a loss function should follow two basic principles:

- If the prediction  $\hat{y}_i$  is *close* to the actual value  $y_i$ , loss should be low.
- If the prediction  $\hat{y}_i$  is *far* from the actual value  $y_i$ , loss should be high.

Two common choices of loss function are squared loss and absolute loss.

**Squared loss**, also known as **L2 loss**, computes loss as the square of the difference between the observed  $y_i$  and predicted  $\hat{y}_i$ :

$$L(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$$

**Absolute loss**, also known as **L1 loss**, computes loss as the absolute difference between the observed  $y_i$  and predicted  $\hat{y}_i$ :

$$L(y_i, \hat{y}_i) = |y_i - \hat{y}_i|$$

L1 and L2 loss give us a tool for quantifying our model’s performance on a single data point. This is a good start, but ideally, we want to understand how our model performs across our *entire* dataset. A natural way to do this is to compute the average loss across all data points in the dataset. This is known as the **cost function**,  $\hat{R}(\theta)$ :

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n L(y_i, \hat{y}_i)$$

The cost function has many names in the statistics literature. You may also encounter the terms:

- Empirical risk (this is why we give the cost function the name  $R$ )
- Error function
- Average loss

We can substitute our L1 and L2 loss into the cost function definition. The **Mean Squared Error (MSE)** is the average squared loss across a dataset:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

The **Mean Absolute Error (MAE)** is the average absolute loss across a dataset:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

## 10.6 Fitting the Model

Now that we've established the concept of a loss function, we can return to our original goal of choosing model parameters. Specifically, we want to choose the best set of model parameters that will minimize the model's cost on our dataset. This process is called fitting the model.

We know from calculus that a function is minimized when (1) its first derivative is equal to zero and (2) its second derivative is positive. We often call the function being minimized the **objective function** (our objective is to find its minimum).

To find the optimal model parameter, we:

1. Take the derivative of the cost function with respect to that parameter
2. Set the derivative equal to 0
3. Solve for the parameter

We repeat this process for each parameter present in the model. For now, we'll disregard the second derivative condition.

To help us make sense of this process, let's put it into action by deriving the optimal model parameters for simple linear regression using the mean squared error as our cost function. Remember: although the notation may look tricky, all we are doing is following the three steps above!

Step 1: take the derivative of the cost function with respect to each model parameter. We substitute the SLR model,  $\hat{y}_i = \theta_0 + \theta_1 x_i$ , into the definition of MSE above and differentiate with respect to  $\theta_0$  and  $\theta_1$ .

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2$$

$$\frac{\partial}{\partial \theta_0} \text{MSE} = \frac{-2}{n} \sum_{i=1}^n y_i - \theta_0 - \theta_1 x_i$$

$$\frac{\partial}{\partial \theta_1} \text{MSE} = \frac{-2}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i) x_i$$

Let's walk through these derivations in more depth, starting with the derivative of MSE with respect to  $\theta_0$ .

Given our MSE above, we know that:

$$\frac{\partial}{\partial \theta_0} \text{MSE} = \frac{\partial}{\partial \theta_0} \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2$$

Noting that the derivative of sum is equivalent to the sum of derivatives, this then becomes:

$$= \frac{1}{n} \sum_{i=1}^n \frac{\partial}{\partial \theta_0} (y_i - \theta_0 - \theta_1 x_i)^2$$

We can then apply the chain rule.

$$= \frac{1}{n} \sum_{i=1}^n 2 \cdot (y_i - \theta_0 - \theta_1 x_i) (-1)$$

Finally, we can simplify the constants, leaving us with our answer.

$$\frac{\partial}{\partial \theta_0} \text{MSE} = \frac{-2}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)$$

Following the same procedure, we can take the derivative of MSE with respect to  $\theta_1$ .

$$\begin{aligned} \frac{\partial}{\partial \theta_1} \text{MSE} &= \frac{\partial}{\partial \theta_1} \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2 \\ &= \frac{1}{n} \sum_{i=1}^n \frac{\partial}{\partial \theta_1} (y_i - \theta_0 - \theta_1 x_i)^2 \\ &= \frac{1}{n} \sum_{i=1}^n 2(y_i - \theta_0 - \theta_1 x_i) (-x_i) \\ &= \frac{-2}{n} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i) x_i \end{aligned}$$



Step 2: set the derivatives equal to 0. After simplifying terms, this produces two **estimating equations**. The best set of model parameters  $(\hat{\theta}_0, \hat{\theta}_1)$  *must* satisfy these two optimality conditions.

$$0 = \frac{-2}{n} \sum_{i=1}^n y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i \iff \frac{1}{n} \sum_{i=1}^n y_i - \hat{y}_i = 0$$

$$0 = \frac{-2}{n} \sum_{i=1}^n (y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i) x_i \iff \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i) x_i = 0$$

Step 3: solve the estimating equations to compute estimates for  $\hat{\theta}_0$  and  $\hat{\theta}_1$ .

Taking the first equation gives the estimate of  $\hat{\theta}_0$ :

$$\frac{1}{n} \sum_{i=1}^n y_i - \hat{\theta}_0 - \hat{\theta}_1 x_i = 0$$

$$\left( \frac{1}{n} \sum_{i=1}^n y_i \right) - \hat{\theta}_0 - \hat{\theta}_1 \left( \frac{1}{n} \sum_{i=1}^n x_i \right) = 0$$

$$\hat{\theta}_0 = \bar{y} - \hat{\theta}_1 \bar{x}$$

With a bit more maneuvering, the second equation gives the estimate of  $\hat{\theta}_1$ . Start by multiplying the first estimating equation by  $\bar{x}$ , then subtracting the result from the second estimating equation.

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i) x_i - \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i) \bar{x} = 0$$

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i) (x_i - \bar{x}) = 0$$

Next, plug in  $\hat{y}_i = \hat{\theta}_0 + \hat{\theta}_1 x_i = \bar{y} + \hat{\theta}_1 (x_i - \bar{x})$ :

$$\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y} - \hat{\theta}_1 (x_i - \bar{x})) (x_i - \bar{x}) = 0$$

$$\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y}) (x_i - \bar{x}) = \hat{\theta}_1 \times \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2$$

By using the definition of correlation  $\left(r = \frac{1}{n} \sum_{i=1}^n \left(\frac{x_i - \bar{x}}{\sigma_x}\right) \left(\frac{y_i - \bar{y}}{\sigma_y}\right)\right)$  and standard deviation  $\left(\sigma_x = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}\right)$ , we can conclude:

$$r\sigma_x\sigma_y = \hat{\theta}_1 \times \sigma_x^2$$

$$\hat{\theta}_1 = r \frac{\sigma_y}{\sigma_x}$$

Just as was given in Data 8!

Remember, this derivation found the optimal model parameters for SLR when using the MSE cost function. If we had used a different model or different loss function, we likely would have found different values for the best model parameters. However, regardless of the model and loss used, we can *always* follow these three steps to fit the model.

## 10.7 Evaluating the SLR Model

Now that we’ve explored the mathematics behind (1) choosing a model, (2) choosing a loss function, and (3) fitting the model, we’re left with one final question – how “good” are the predictions made by this “best” fitted model? To determine this, we can:

1. Visualize data and compute statistics:

- Plot the original data.
- Compute each column’s mean and standard deviation. If the mean and standard deviation of our predictions are close to those of the original observed  $y_i$ ’s, we might be inclined to say that our model has done well.
- (If we’re fitting a linear model) Compute the correlation  $r$ . A large magnitude for the correlation coefficient between the feature and response variables could also indicate that our model has done well.

2. Performance metrics:

- We can take the **Root Mean Squared Error (RMSE)**.
  - It’s the square root of the mean squared error (MSE), which is the average loss that we’ve been minimizing to determine optimal model parameters.
  - RMSE is in the same units as  $y$ .
  - A lower RMSE indicates more “accurate” predictions, as we have a lower “average loss” across the data.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

### 3. Visualization:

- Look at the residual plot of  $e_i = y_i - \hat{y}_i$  to visualize the difference between actual and predicted values. The good residual plot should not show any pattern between input/features  $x_i$  and residual values  $e_i$ .

To illustrate this process, let's take a look at **Anscombe's quartet**.

#### 10.7.1 Four Mysterious Datasets (Anscombe's quartet)

Let's take a look at four different datasets.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
import itertools
from mpl_toolkits.mplot3d import Axes3D

# Big font helper
def adjust_fontsize(size=None):
    SMALL_SIZE = 8
    MEDIUM_SIZE = 10
    BIGGER_SIZE = 12
    if size != None:
        SMALL_SIZE = MEDIUM_SIZE = BIGGER_SIZE = size

    plt.rc("font", size=SMALL_SIZE) # controls default text sizes
    plt.rc("axes", titlesize=SMALL_SIZE) # fontsize of the axes title
    plt.rc("axes", labelsiz=SMALL_SIZE) # fontsize of the x and y labels
    plt.rc("xtick", labelsiz=SMALL_SIZE) # fontsize of the tick labels
    plt.rc("ytick", labelsiz=SMALL_SIZE) # fontsize of the tick labels
    plt.rc("legend", fontsize=SMALL_SIZE) # legend fontsize
    plt.rc("figure", titlesize=BIGGER_SIZE) # fontsize of the figure title

# Helper functions
def standard_units(x):
    return (x - np.mean(x)) / np.std(x)
```

```

def correlation(x, y):
    return np.mean(standard_units(x) * standard_units(y))

def slope(x, y):
    return correlation(x, y) * np.std(y) / np.std(x)

def intercept(x, y):
    return np.mean(y) - slope(x, y) * np.mean(x)

def fit_least_squares(x, y):
    theta_0 = intercept(x, y)
    theta_1 = slope(x, y)
    return theta_0, theta_1

def predict(x, theta_0, theta_1):
    return theta_0 + theta_1 * x

def compute_mse(y, yhat):
    return np.mean((y - yhat) ** 2)

plt.style.use("default") # Revert style to default mpl

plt.style.use("default") # Revert style to default mpl
NO_VIZ, RESID, RESID_SCATTER = range(3)

def least_squares_evaluation(x, y, visualize=NO_VIZ):
    # statistics
    print(f"x_mean : {np.mean(x):.2f}, y_mean : {np.mean(y):.2f}")
    print(f"x_stdev: {np.std(x):.2f}, y_stdev: {np.std(y):.2f}")
    print(f"r = Correlation(x, y): {correlation(x, y):.3f}")

    # Performance metrics
    ahat, bhat = fit_least_squares(x, y)
    yhat = predict(x, ahat, bhat)
    print(f"\theta_0: {ahat:.2f}, \theta_1: {bhat:.2f}")

```

```

print(f"RMSE: {np.sqrt(compute_mse(y, yhat)):.3f}")

# visualization
fig, ax_resid = None, None
if visualize == RESID_SCATTER:
    fig, axs = plt.subplots(1, 2, figsize=(8, 3))
    axs[0].scatter(x, y)
    axs[0].plot(x, yhat)
    axs[0].set_title("LS fit")
    ax_resid = axs[1]
elif visualize == RESID:
    fig = plt.figure(figsize=(4, 3))
    ax_resid = plt.gca()

if ax_resid is not None:
    ax_resid.scatter(x, y - yhat, color="red")
    ax_resid.plot([4, 14], [0, 0], color="black")
    ax_resid.set_title("Residuals")

return fig

```

```

# Load in four different datasets: I, II, III, IV
x = [10, 8, 13, 9, 11, 14, 6, 4, 12, 7, 5]
y1 = [8.04, 6.95, 7.58, 8.81, 8.33, 9.96, 7.24, 4.26, 10.84, 4.82, 5.68]
y2 = [9.14, 8.14, 8.74, 8.77, 9.26, 8.10, 6.13, 3.10, 9.13, 7.26, 4.74]
y3 = [7.46, 6.77, 12.74, 7.11, 7.81, 8.84, 6.08, 5.39, 8.15, 6.42, 5.73]
x4 = [8, 8, 8, 8, 8, 8, 8, 19, 8, 8, 8]
y4 = [6.58, 5.76, 7.71, 8.84, 8.47, 7.04, 5.25, 12.50, 5.56, 7.91, 6.89]

anscombe = {
    "I": pd.DataFrame(list(zip(x, y1)), columns=["x", "y"]),
    "II": pd.DataFrame(list(zip(x, y2)), columns=["x", "y"]),
    "III": pd.DataFrame(list(zip(x, y3)), columns=["x", "y"]),
    "IV": pd.DataFrame(list(zip(x4, y4)), columns=["x", "y"]),
}

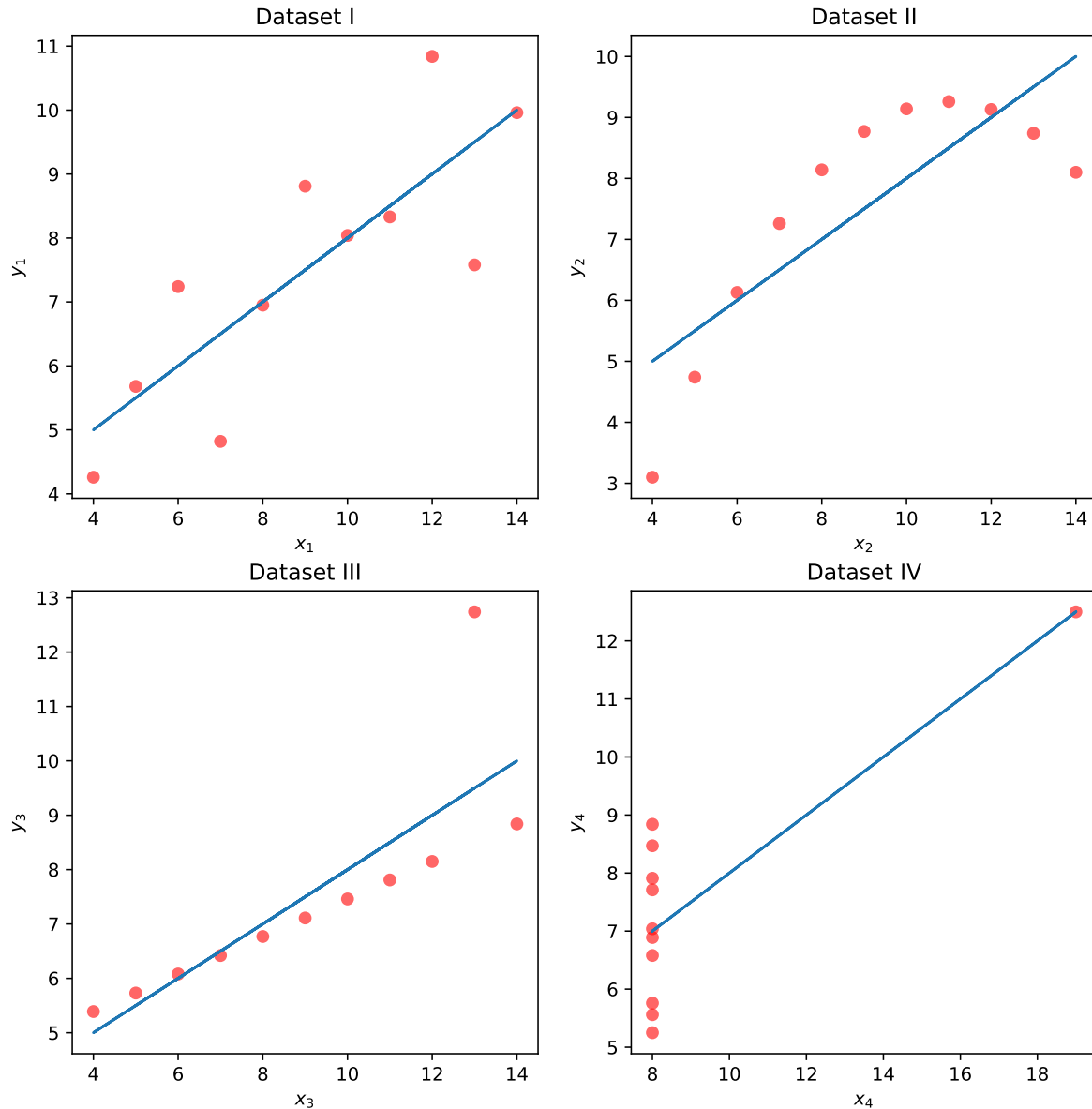
# Plot the scatter plot and line of best fit
fig, axs = plt.subplots(2, 2, figsize=(10, 10))

for i, dataset in enumerate(["I", "II", "III", "IV"]):
    ans = anscombe[dataset]
    x, y = ans["x"], ans["y"]

```

```
ahat, bhat = fit_least_squares(x, y)
yhat = predict(x, ahat, bhat)
axs[i // 2, i % 2].scatter(x, y, alpha=0.6, color="red") # plot the x, y points
axs[i // 2, i % 2].plot(x, yhat) # plot the line of best fit
axs[i // 2, i % 2].set_xlabel(f"$x_{i+1}$")
axs[i // 2, i % 2].set_ylabel(f"$y_{i+1}$")
axs[i // 2, i % 2].set_title(f"Dataset {dataset}")

plt.show()
```



While these four sets of datapoints look very different, they actually all have identical means  $\bar{x}$ ,  $\bar{y}$ , standard deviations  $\sigma_x$ ,  $\sigma_y$ , correlation  $r$ , and RMSE! If we only look at these statistics, we would probably be inclined to say that these datasets are similar.

```
for dataset in ["I", "II", "III", "IV"]:
    print(f">>> Dataset {dataset}:")
    ans = anscombe[dataset]
    fig = least_squares_evaluation(ans["x"], ans["y"], visualize=NO_VIZ)
```

```
print()
print()
```

```
>>> Dataset I:
x_mean : 9.00, y_mean : 7.50
x_stdev: 3.16, y_stdev: 1.94
r = Correlation(x, y): 0.816
    heta_0: 3.00,    heta_1: 0.50
RMSE: 1.119
```

```
>>> Dataset II:
x_mean : 9.00, y_mean : 7.50
x_stdev: 3.16, y_stdev: 1.94
r = Correlation(x, y): 0.816
    heta_0: 3.00,    heta_1: 0.50
RMSE: 1.119
```

```
>>> Dataset III:
x_mean : 9.00, y_mean : 7.50
x_stdev: 3.16, y_stdev: 1.94
r = Correlation(x, y): 0.816
    heta_0: 3.00,    heta_1: 0.50
RMSE: 1.118
```

```
>>> Dataset IV:
x_mean : 9.00, y_mean : 7.50
x_stdev: 3.16, y_stdev: 1.94
r = Correlation(x, y): 0.817
    heta_0: 3.00,    heta_1: 0.50
RMSE: 1.118
```

We may also wish to visualize the model's **residuals**, defined as the difference between the observed and predicted  $y_i$  value ( $e_i = y_i - \hat{y}_i$ ). This gives a high-level view of how “off” each prediction is from the true observed value. Recall that you explored this concept in [Data 8](#): a good regression fit should display no clear pattern in its plot of residuals. The residual plots for Anscombe's quartet are displayed below. Note how only the first plot shows no clear pattern to the magnitude of residuals. This is an indication that SLR is not the best choice of model for the remaining three sets of points.



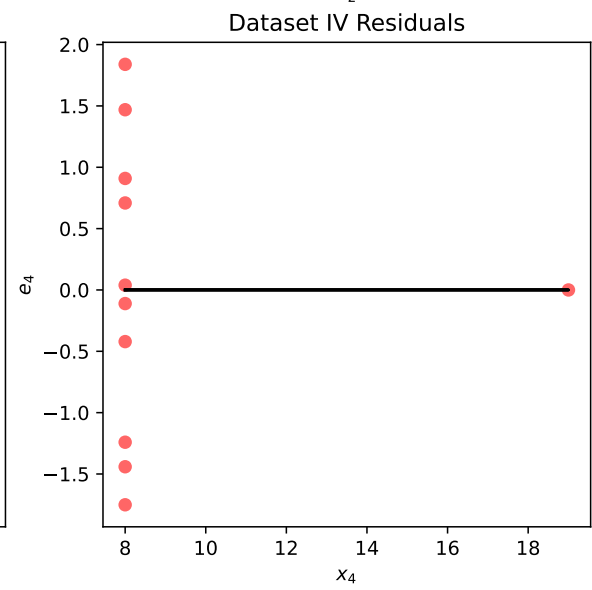
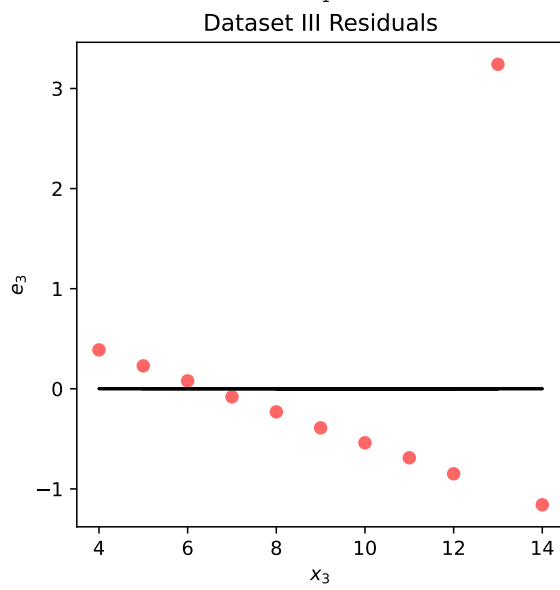
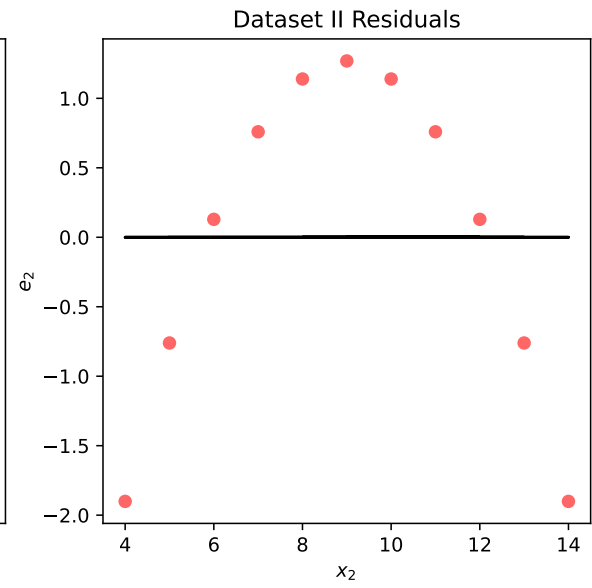
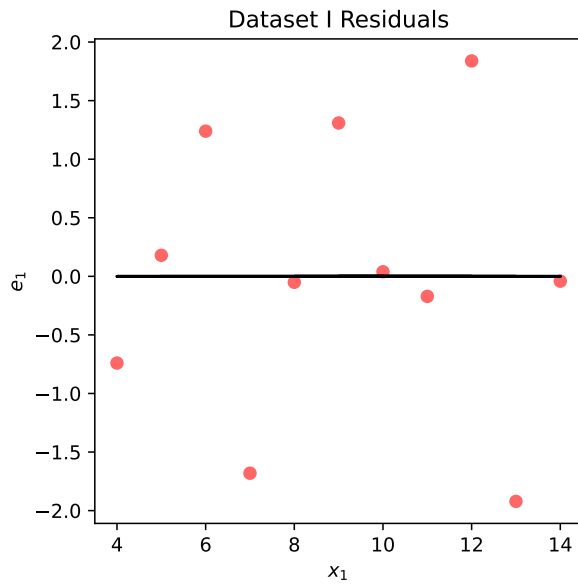
```

# Residual visualization
fig, axs = plt.subplots(2, 2, figsize=(10, 10))

for i, dataset in enumerate(["I", "II", "III", "IV"]):
    ans = anscombe[dataset]
    x, y = ans["x"], ans["y"]
    ahat, bhat = fit_least_squares(x, y)
    yhat = predict(x, ahat, bhat)
    axs[i // 2, i % 2].scatter(
        x, y - yhat, alpha=0.6, color="red"
    ) # plot the x, y points
    axs[i // 2, i % 2].plot(
        x, np.zeros_like(x), color="black"
    ) # plot the residual line
    axs[i // 2, i % 2].set_xlabel(f"$x_{i+1}$")
    axs[i // 2, i % 2].set_ylabel(f"$e_{i+1}$")
    axs[i // 2, i % 2].set_title(f"Dataset {dataset} Residuals")

plt.show()

```



# 11 Constant Model, Loss, and Transformations

## Learning Outcomes

- Derive the optimal model parameters for the constant model under MSE and MAE cost functions.
- Evaluate the differences between MSE and MAE risk.
- Understand the need for linearization of variables and apply the Tukey-Mosteller bulge diagram for transformations.

Last time, we introduced the modeling process. We set up a framework to predict target variables as functions of our features, following a set workflow:

1. Choose a model - how should we represent the world?
2. Choose a loss function - how do we quantify prediction error?
3. Fit the model - how do we choose the best parameter of our model given our data?
4. Evaluate model performance - how do we evaluate whether this process gave rise to a good model?

To illustrate this process, we derived the optimal model parameters under simple linear regression (SLR) with mean squared error (MSE) as the cost function. A summary of the SLR modeling process is shown below:

At the end of last lecture, we dived deeper into step 4 - evaluating model performance - using SLR as an example. In this lecture, we'll also explore the modeling process with new models, continue familiarizing ourselves with the modeling process by finding the best model parameters under a new model, the constant model, and test out two different loss functions to understand how our choice of loss influences model design. Later on, we'll consider what happens when a linear model isn't the best choice to capture trends in our data and what solutions there are to create better models.

Before we get into the modeling process, let's quickly review some important terminology.

## 11.1 Constant Model + MSE

Now, we'll shift from the SLR model to the **constant model**, also known as a summary statistic. The constant model is slightly different from the simple linear regression model we've

explored previously. Rather than generating predictions from an inputted feature variable, the constant model always *predicts the same constant number*. This ignores any relationships between variables. For example, let's say we want to predict the number of drinks a boba shop sells in a day. Boba tea sales likely depend on the time of year, the weather, how the customers feel, whether school is in session, etc., but the constant model ignores these factors in favor of a simpler model. In other words, the constant model employs a **simplifying assumption**.

It is also a parametric, statistical model:

$$\hat{y} = \theta_0$$

$\theta_0$  is the parameter of the constant model, just as  $\theta_0$  and  $\theta_1$  were the parameters in SLR. Since our parameter  $\theta_0$  is 1-dimensional ( $\theta_0 \in \mathbb{R}$ ), we now have no input to our model and will always predict  $\hat{y} = \theta_0$ .

### 11.1.1 Deriving the optimal $\theta_0$

Our task now is to determine what value of  $\theta_0$  best represents the optimal model – in other words, what number should we guess each time to have the lowest possible **average loss** on our data?

Like before, we'll use Mean Squared Error (MSE). Recall that the MSE is average squared loss (L2 loss) over the data  $D = \{y_1, y_2, \dots, y_n\}$ .

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Our modeling process now looks like this:

1. Choose a model: constant model
2. Choose a loss function: L2 loss
3. Fit the model
4. Evaluate model performance

Given the **constant model**  $\hat{y} = \theta_0$ , we can rewrite the MSE equation as

$$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0)^2$$

We can **fit the model** by finding the optimal  $\hat{\theta}_0$  that minimizes the MSE using a calculus approach.

1. Differentiate with respect to  $\theta_0$ :

$$\frac{d}{d\theta_0}R(\theta) = \frac{d}{d\theta_0}\left(\frac{1}{n}\sum_{i=1}^n(y_i - \theta_0)^2\right) \quad (11.1)$$

$$= \frac{1}{n}\sum_{i=1}^n \frac{d}{d\theta_0}(y_i - \theta_0)^2 \quad \text{a derivative of sum is a sum of derivatives} \quad (11.2)$$

$$= \frac{1}{n}\sum_{i=1}^n 2(y_i - \theta_0)(-1) \quad \text{chain rule} \quad (11.3)$$

$$= \frac{-2}{n}\sum_{i=1}^n(y_i - \theta_0) \quad \text{simplify constants} \quad (11.4)$$

2. Set the derivative equation equal to 0:

$$0 = \frac{-2}{n}\sum_{i=1}^n(y_i - \hat{\theta}_0)$$

3. Solve for  $\hat{\theta}_0$

$$0 = \frac{-2}{n}\sum_{i=1}^n(y_i - \hat{\theta}_0) \quad (11.5)$$

$$= \sum_{i=1}^n(y_i - \hat{\theta}_0) \quad \text{divide both sides by } \frac{-2}{n} \quad (11.6)$$

$$= \left(\sum_{i=1}^n y_i\right) - \left(\sum_{i=1}^n \hat{\theta}_0\right) \quad \text{separate sums} \quad (11.7)$$

$$= \left(\sum_{i=1}^n y_i\right) - (n \cdot \hat{\theta}_0) \quad \text{c} + \text{c} + \dots + \text{c} = \text{nc} \quad (11.8)$$

$$n \cdot \hat{\theta}_0 = \sum_{i=1}^n y_i \quad (11.9)$$

$$\hat{\theta}_0 = \frac{1}{n}\sum_{i=1}^n y_i \quad (11.10)$$

$$\hat{\theta}_0 = \bar{y} \quad (11.11)$$

**i** Note

The **mean** of the outcomes achieves the minimum MSE of the constant model. Minimum MSE is the **sample variance** of  $y$

$$R(\hat{\theta}_0) = R(\bar{y}) \quad (11.12)$$

$$= \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 \quad (11.13)$$

$$= \sigma_y^2 \quad (11.14)$$

$R^2$  is interpreted as the fraction of **variance in  $y$**  “explained” by a linear model.

$$R^2 = \frac{\Delta \text{ in area}}{\text{Constant model area}} \quad (11.15)$$

$$(11.16)$$

$$= \frac{\text{MSE}_{\text{constant model}} - \text{MSE}_{\text{linear model}}}{\text{MSE}_{\text{constant model}}} \quad (11.17)$$

Let’s take a moment to interpret this result.  $\hat{\theta}_0 = \bar{y}$  is the optimal parameter for constant model + MSE. It holds true regardless of what data sample you have, and it provides some formal reasoning as to why the mean is such a common summary statistic.

Our optimal model parameter is the value of the parameter that minimizes the cost function. This minimum value of the cost function can be expressed:

$$R(\hat{\theta}_0) = \min_{\theta_0} R(\theta_0)$$

To restate the above in plain English: we are looking at the value of the cost function when it takes the best parameter as input. This optimal model parameter,  $\hat{\theta}_0$ , is the value of  $\theta_0$  that minimizes the cost  $R$ .

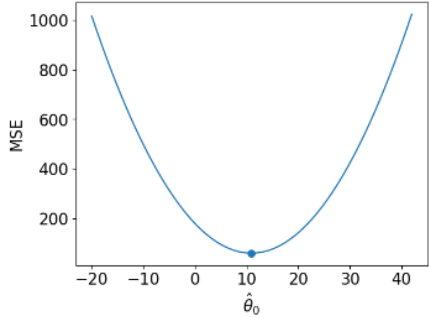
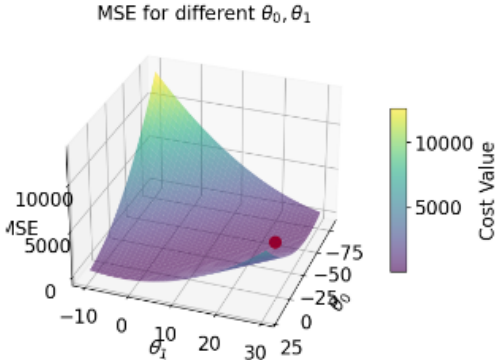
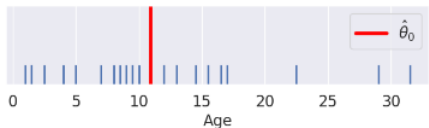
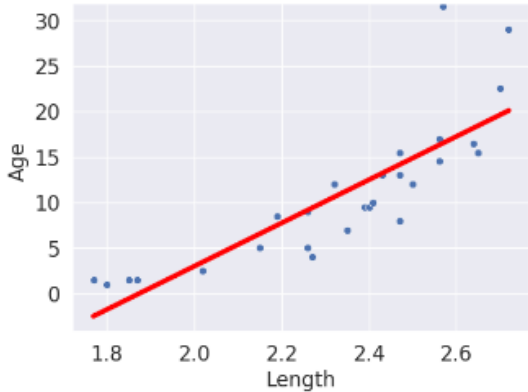
For modeling purposes, we care less about the minimum value of cost,  $R(\hat{\theta}_0)$ , and more about the *value of  $\theta_0$*  that results in this lowest average loss. In other words, we concern ourselves with finding the best parameter value such that:

$$\hat{\theta}_0 = \arg \min_{\theta_0} R(\theta_0)$$

That is, we want to find the **argument**  $\theta_0$  that **minimizes** the cost function.

### 11.1.2 Comparing Two Different Models, Both Fit with MSE

Now that we've explored the constant model with an L2 loss, we can compare it to the SLR model that we learned last lecture. Consider the dataset below, which contains information about the ages and lengths of dugongs. Supposed we wanted to predict dugong ages:

	Constant Model	Simple Linear Regression
model	$\hat{y} = \theta_0$	$\hat{y} = \theta_0 + \theta_1 x$
data	sample of ages $D = \{y_1, y_2, \dots, y_n\}$	sample of ages $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
dimensions	$\hat{\theta}_0$ is 1-D	$\hat{\theta} = [\hat{\theta}_0, \hat{\theta}_1]$ is 2-D
loss surface	2-D 	3-D 
loss model	$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0)^2$	$\hat{R}(\theta_0, \theta_1) = \frac{1}{n} \sum_{i=1}^n (y_i - (\theta_0 + \theta_1 x))^2$
RMSE	7.72	4.31
predictions visualized	rug plot 	scatter plot 

(Notice how the points for our SLR scatter plot are visually not a great linear fit. We'll come back to this).

The code for generating the graphs and models is included below, but we won't go over it in too much depth.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
import itertools
from mpl_toolkits.mplot3d import Axes3D
dugongs = pd.read_csv("data/dugongs.csv")
data_constant = dugongs["Age"]
data_linear = dugongs[["Length", "Age"]]
```

```
# Big font helper
def adjust_fontsize(size=None):
    SMALL_SIZE = 8
    MEDIUM_SIZE = 10
    BIGGER_SIZE = 12
    if size != None:
        SMALL_SIZE = MEDIUM_SIZE = BIGGER_SIZE = size

    plt.rc("font", size=SMALL_SIZE) # controls default text sizes
    plt.rc("axes", titlesize=SMALL_SIZE) # fontsize of the axes title
    plt.rc("axes", labelsiz=SMALL_SIZE) # fontsize of the x and y labels
    plt.rc("xtick", labelsiz=SMALL_SIZE) # fontsize of the tick labels
    plt.rc("ytick", labelsiz=SMALL_SIZE) # fontsize of the tick labels
    plt.rc("legend", fontsize=SMALL_SIZE) # legend fontsize
    plt.rc("figure", titlesize=BIGGER_SIZE) # fontsize of the figure title

plt.style.use("default") # Revert style to default mpl
```

```
# Constant Model + MSE
plt.style.use('default') # Revert style to default mpl
adjust_fontsize(size=16)
%matplotlib inline

def mse_constant(theta, data):
    return np.mean(np.array([(y_obs - theta) ** 2 for y_obs in data]), axis=0)

thetas = np.linspace(-20, 42, 1000)
l2_loss_thetas = mse_constant(thetas, data_constant)
```

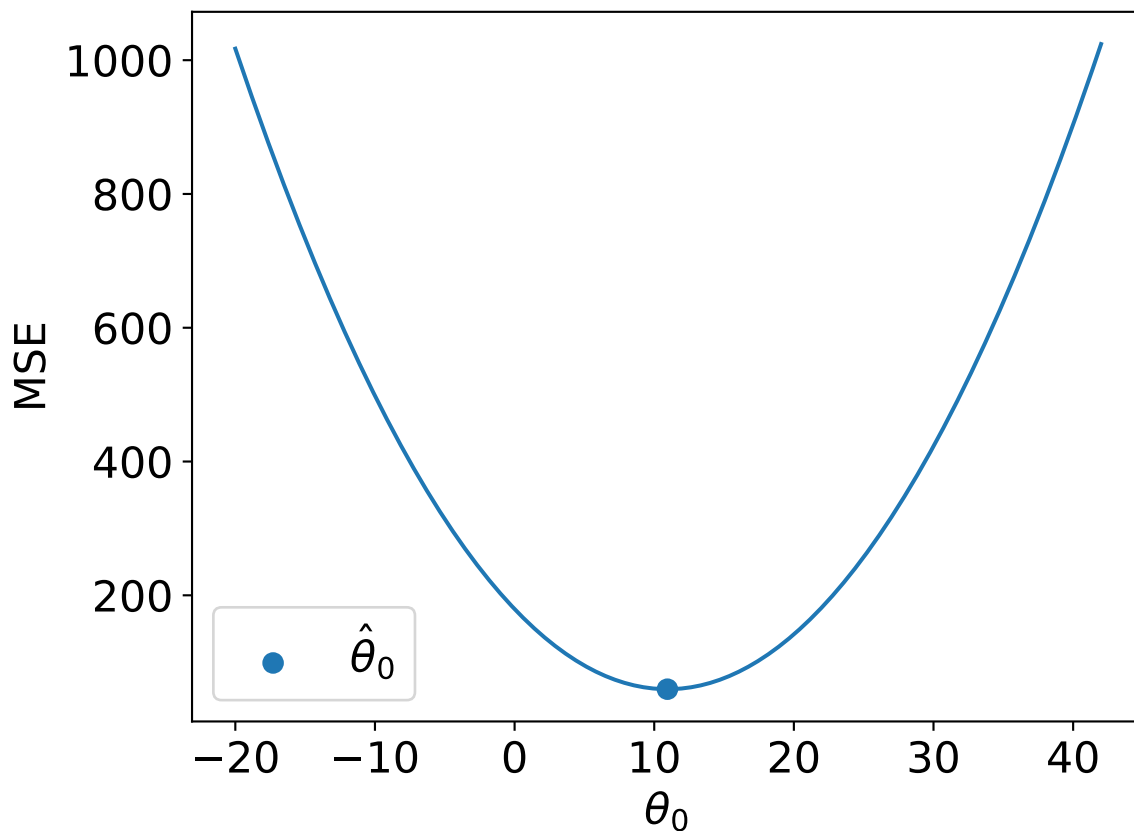


```

# Plotting the loss surface
plt.plot(thetas, l2_loss_thetas)
plt.xlabel(r'$\theta_0$')
plt.ylabel(r'MSE')

# Optimal point
thetahat = np.mean(data_constant)
plt.scatter([thetahat], [mse_constant(thetahat, data_constant)], s=50, label = r"$\hat{\theta}_0$")
plt.legend();
# plt.show()

```



```

# SLR + MSE
def mse_linear(theta_0, theta_1, data_linear):
    data_x, data_y = data_linear.iloc[:, 0], data_linear.iloc[:, 1]
    return np.mean(
        np.array([(y - (theta_0 + theta_1 * x)) ** 2 for x, y in zip(data_x, data_y)]),

```

```

        axis=0,
    )

# plotting the loss surface
theta_0_values = np.linspace(-80, 20, 80)
theta_1_values = np.linspace(-10, 30, 80)
mse_values = np.array(
    [[mse_linear(x, y, data_linear) for x in theta_0_values] for y in theta_1_values]
)

# Optimal point
data_x, data_y = data_linear.iloc[:, 0], data_linear.iloc[:, 1]
theta_1_hat = np.corrcoef(data_x, data_y)[0, 1] * np.std(data_y) / np.std(data_x)
theta_0_hat = np.mean(data_y) - theta_1_hat * np.mean(data_x)

# Create the 3D plot
fig = plt.figure(figsize=(7, 5))
ax = fig.add_subplot(111, projection="3d")

X, Y = np.meshgrid(theta_0_values, theta_1_values)
surf = ax.plot_surface(
    X, Y, mse_values, cmap="viridis", alpha=0.6
) # Use alpha to make it slightly transparent

# Scatter point using matplotlib
sc = ax.scatter(
    [theta_0_hat],
    [theta_1_hat],
    [mse_linear(theta_0_hat, theta_1_hat, data_linear)],
    marker="o",
    color="red",
    s=100,
    label="theta hat",
)

# Create a colorbar
cbar = fig.colorbar(surf, ax=ax, shrink=0.5, aspect=10)
cbar.set_label("Cost Value")

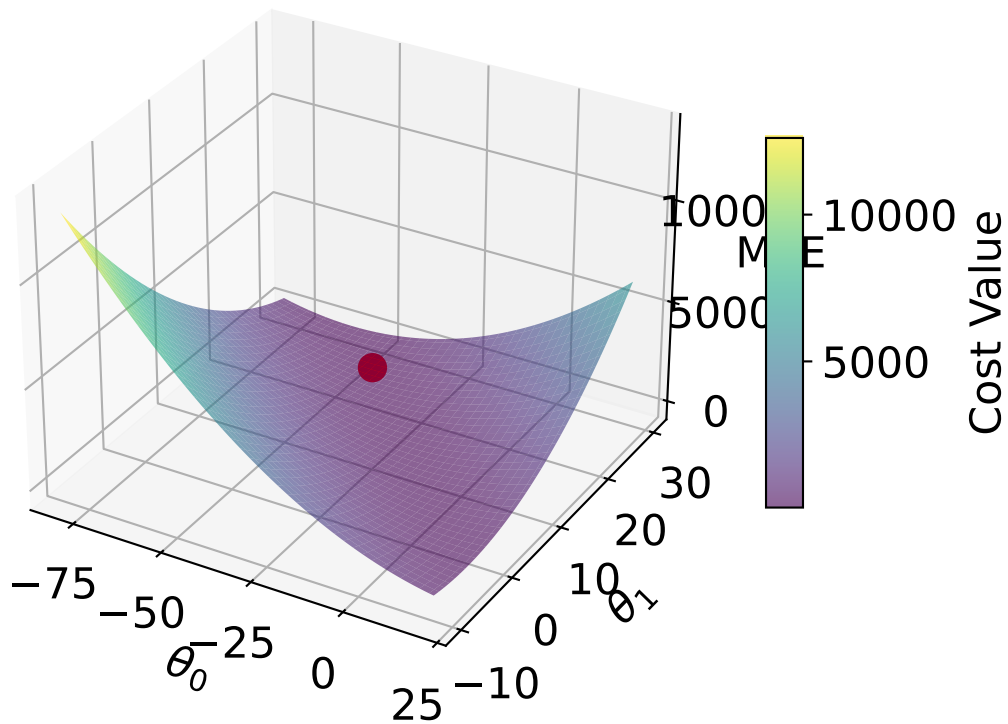
ax.set_title("MSE for different  $\theta_0$ ,  $\theta_1$ ")
ax.set_xlabel(" $\theta_0$ ")

```

```
ax.set_ylabel("$\\theta_1$")
ax.set_zlabel("MSE");

# plt.show()
```

MSE for different  $\theta_0, \theta_1$



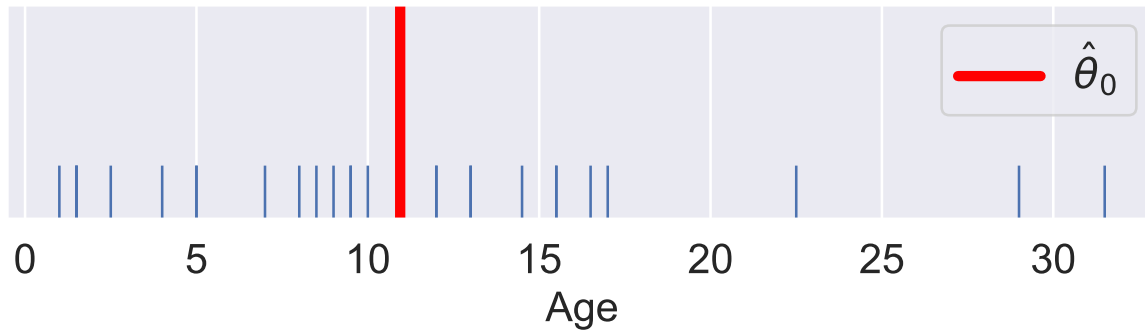
```
# Predictions
yobs = data_linear["Age"] # The true observations y
xs = data_linear["Length"] # Needed for linear predictions
n = len(yobs) # Predictions

yhats_constant = [thetahat for i in range(n)] # Not used, but food for thought
yhats_linear = [theta_0_hat + theta_1_hat * x for x in xs]

# Constant Model Rug Plot
# In case we're in a weird style state
sns.set_theme()
adjust_fontsize(size=16)
```

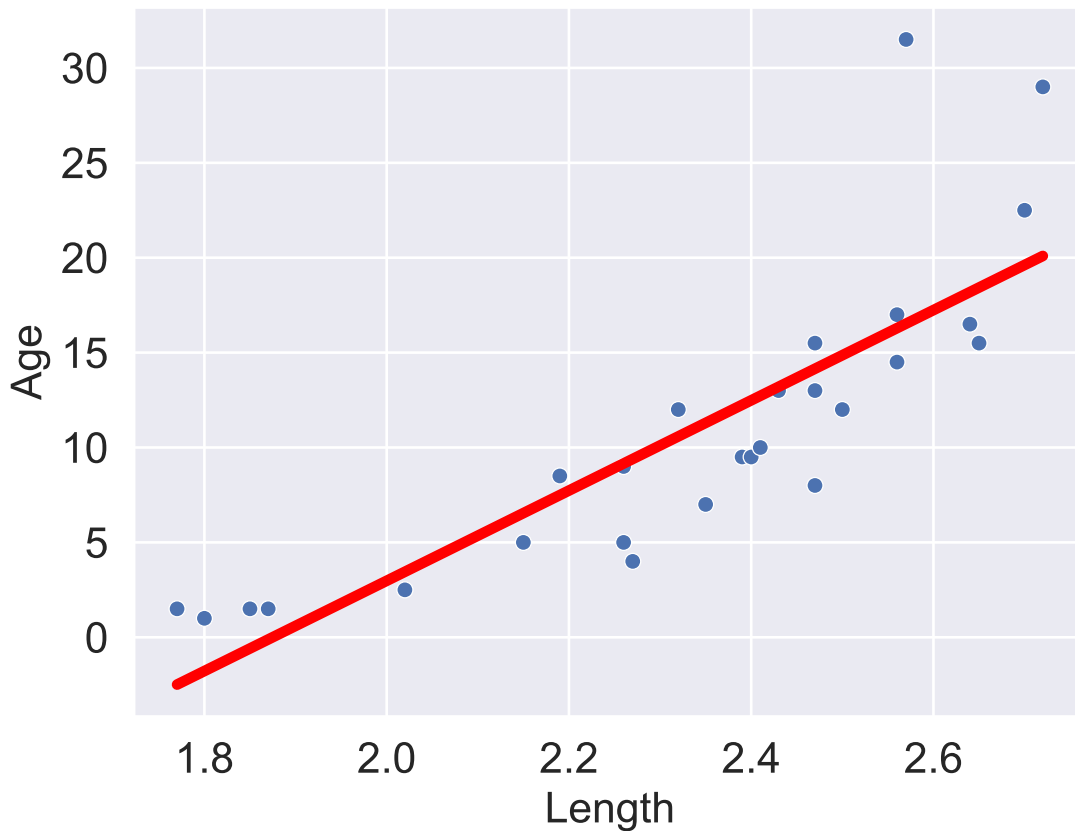
```
%matplotlib inline
```

```
fig = plt.figure(figsize=(8, 1.5))
sns.rugplot(yobs, height=0.25, lw=2) ;
plt.axvline(thetahat, color='red', lw=4, label=r"$\hat{\theta}_0$");
plt.legend()
plt.yticks([]);
# plt.show()
```



```
# SLR model scatter plot
# In case we're in a weird style state
sns.set_theme()
adjust_fontsize(size=16)
%matplotlib inline

sns.scatterplot(x=xs, y=yobs)
plt.plot(xs, yhats_linear, color='red', lw=4);
# plt.savefig('dugong_line.png', bbox_inches = 'tight');
# plt.show()
```



Interpreting the RMSE (Root Mean Squared Error):

- Because the constant error is **HIGHER** than the linear error,
- The constant model is **WORSE** than the linear model (at least for this metric).

## 11.2 Constant Model + MAE

We see now that changing the model used for prediction leads to a wildly different result for the optimal model parameter. What happens if we instead change the loss function used in model evaluation?

This time, we will consider the constant model with L1 (absolute loss) as the loss function. This means that the average loss will be expressed as the **Mean Absolute Error (MAE)**.

1. Choose a model: constant model
2. Choose a loss function: L1 loss
3. Fit the model
4. Evaluate model performance

### 11.2.1 Deriving the optimal $\theta_0$

Recall that the MAE is average **absolute** loss (L1 loss) over the data  $D = \{y_1, y_2, \dots, y_n\}$ .

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

Given the constant model  $\hat{y} = \theta_0$ , we can write the MAE as:

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^n |y_i - \theta_0|$$

To fit the model, we find the optimal parameter value  $\hat{\theta}_0$  that minimizes the MAE by differentiating using a calculus approach:

1. Differentiate with respect to  $\hat{\theta}_0$ :

$$\hat{R}(\theta_0) = \frac{1}{n} \sum_{i=1}^n |y_i - \theta_0| \tag{11.18}$$

$$\frac{d}{d\theta_0} R(\theta_0) = \frac{d}{d\theta_0} \left( \frac{1}{n} \sum_{i=1}^n |y_i - \theta_0| \right) \tag{11.19}$$

$$= \frac{1}{n} \sum_{i=1}^n \frac{d}{d\theta_0} |y_i - \theta_0| \tag{11.20}$$

- Here, we seem to have run into a problem: the derivative of an absolute value is undefined when the argument is 0 (i.e. when  $y_i = \theta_0$ ). For now, we'll ignore this issue. It turns out that disregarding this case doesn't influence our final result.
- To perform the derivative, consider two cases. When  $\theta_0$  is *less than or equal to*  $y_i$ , the term  $y_i - \theta_0$  will be positive and the absolute value has no impact. When  $\theta_0$  is *greater than*  $y_i$ , the term  $y_i - \theta_0$  will be negative. Applying the absolute value will convert this to a positive value, which we can express by saying  $-(y_i - \theta_0) = \theta_0 - y_i$ .

$$|y_i - \theta_0| = \begin{cases} y_i - \theta_0 & \text{if } \theta_0 \leq y_i \\ \theta_0 - y_i & \text{if } \theta_0 > y_i \end{cases}$$

- Taking derivatives:

$$\frac{d}{d\theta_0}|y_i - \theta_0| = \begin{cases} \frac{d}{d\theta_0}(y_i - \theta_0) = -1 & \text{if } \theta_0 < y_i \\ \frac{d}{d\theta_0}(\theta_0 - y_i) = 1 & \text{if } \theta_0 > y_i \end{cases}$$

- This means that we obtain a different value for the derivative for data points where  $\theta_0 < y_i$  and where  $\theta_0 > y_i$ . We can summarize this by saying:

$$\frac{d}{d\theta_0}R(\theta_0) = \frac{1}{n} \sum_{i=1}^n \frac{d}{d\theta_0}|y_i - \theta_0| = \frac{1}{n} \left[ \sum_{\theta_0 < y_i} (-1) + \sum_{\theta_0 > y_i} (+1) \right]$$

- In other words, we take the sum of values for  $i = 1, 2, \dots, n$ :
  - $-1$  if our observation  $y_i$  is *greater than* our prediction  $\hat{\theta}_0$
  - $+1$  if our observation  $y_i$  is *smaller than* our prediction  $\hat{\theta}_0$

2. Set the derivative equation equal to 0:

$$0 = \frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (-1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (+1)$$

3. Solve for  $\hat{\theta}_0$ :

$$0 = -\frac{1}{n} \sum_{\hat{\theta}_0 < y_i} (1) + \frac{1}{n} \sum_{\hat{\theta}_0 > y_i} (1)$$

$$\sum_{\hat{\theta}_0 < y_i} (1) = \sum_{\hat{\theta}_0 > y_i} (1)$$

Thus, the constant model parameter  $\theta = \hat{\theta}_0$  that minimizes MAE must satisfy:

$$\sum_{\hat{\theta}_0 < y_i} (1) = \sum_{\hat{\theta}_0 > y_i} (1)$$

In other words, the number of observations greater than  $\theta_0$  must be equal to the number of observations less than  $\theta_0$ ; there must be an equal number of points on the left and right sides of the equation. This is the definition of median, so our optimal value is

$$\hat{\theta}_0 = \text{median}(y)$$

## 11.3 Summary: Loss Optimization, Calculus, and Critical Points

First, define the **objective function** as average loss.

- Plug in L1 or L2 loss.
- Plug in the model so that the resulting expression is a function of  $\theta$ .

Then, find the minimum of the objective function:

1. Differentiate with respect to  $\theta$ .
2. Set equal to 0.
3. Solve for  $\hat{\theta}$ .
4. (If we have multiple parameters) repeat steps 1-3 with partial derivatives.

Recall critical points from calculus:  $R(\hat{\theta})$  could be a minimum, maximum, or saddle point!

- We should technically also perform the second derivative test, i.e., show  $R''(\hat{\theta}) > 0$ .
- MSE has a property—**convexity**—that guarantees that  $R(\hat{\theta})$  is a global minimum.
- The proof of convexity for MAE is beyond this course.

## 11.4 Comparing Loss Functions

We've now tried our hand at fitting a model under both MSE and MAE cost functions. How do the two results compare?

Let's consider a dataset where each entry represents the number of drinks sold at a bubble tea store each day. We'll fit a constant model to predict the number of drinks that will be sold tomorrow.

```
drinks = np.array([20, 21, 22, 29, 33])
drinks
```

```
array([20, 21, 22, 29, 33])
```

From our derivations above, we know that the optimal model parameter under MSE cost is the mean of the dataset. Under MAE cost, the optimal parameter is the median of the dataset.

```
np.mean(drinks), np.median(drinks)
```

```
(np.float64(25.0), np.float64(22.0))
```



If we plot each empirical risk function across several possible values of  $\theta$ , we find that each  $\hat{\theta}$  does indeed correspond to the lowest value of error:

Notice that the MSE above is a **smooth** function – it is differentiable at all points, making it easy to minimize using numerical methods. The MAE, in contrast, is not differentiable at each of its “kinks.” We’ll explore how the smoothness of the cost function can impact our ability to apply numerical optimization in a few weeks.

How do outliers affect each cost function? Imagine we replace the largest value in the dataset with 1000. The mean of the data increases substantially, while the median is nearly unaffected.

```
drinks_with_outlier = np.append(drinks, 1033)
display(drinks_with_outlier)
np.mean(drinks_with_outlier), np.median(drinks_with_outlier)
```

```
array([ 20,  21,  22,  29,  33, 1033])
```

```
(np.float64(193.0), np.float64(25.5))
```

This means that under the MSE, the optimal model parameter  $\hat{\theta}$  is strongly affected by the presence of outliers. Under the MAE, the optimal parameter is not as influenced by outlying data. We can generalize this by saying that the MSE is **sensitive** to outliers, while the MAE is **robust** to outliers.

Let’s try another experiment. This time, we’ll add an additional, non-outlying datapoint to the data.

```
drinks_with_additional_observation = np.append(drinks, 35)
drinks_with_additional_observation
```

```
array([20, 21, 22, 29, 33, 35])
```

When we again visualize the cost functions, we find that the MAE now plots a horizontal line between 22 and 29. This means that there are *infinitely* many optimal values for the model parameter: any value  $\hat{\theta} \in [22, 29]$  will minimize the MAE. In contrast, the MSE still has a single best value for  $\hat{\theta}$ . In other words, the MSE has a **unique** solution for  $\hat{\theta}$ ; the MAE is not guaranteed to have a single unique solution.

To summarize our example,

	MSE (Mean Squared Loss)	MAE (Mean Absolute Loss)
Loss Function	$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \theta_0)^2$	$\hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^n  y_i - \theta_0 $
Optimal $\hat{\theta}_0$	$\hat{\theta}_0 = \text{mean}(y) = \bar{y}$	$\hat{\theta}_0 = \text{median}(y)$
Loss Surface		
Shape	<b>Smooth</b> - easy to minimize using numerical methods (in a few weeks)	<b>Piecewise</b> - at each of the “kinks,” it’s not differentiable. Harder to minimize.
Outliers	<b>Sensitive</b> to outliers (since they change mean substantially). Sensitivity also depends on the dataset size.	<b>More robust</b> to outliers.
$\hat{\theta}_0$ Uniqueness	<b>Unique</b> $\hat{\theta}_0$	<b>Infinitely many</b> $\hat{\theta}_0$ s

## 11.5 Transformations of Linear Models

At this point, we have an effective method of fitting models to predict linear relationships. Given a feature variable and target, we can apply our four-step process to find the optimal model parameters.

A key word above is *linear*. When we computed parameter estimates earlier, we assumed that  $x_i$  and  $y_i$  shared a roughly linear relationship. Data in the real world isn’t always so straightforward, but we can transform the data to try and obtain linearity.

The **Tukey-Mosteller Bulge Diagram** is a useful tool for summarizing what transformations can linearize the relationship between two variables. To determine what transformations might be appropriate, trace the shape of the “bulge” made by your data. Find the quadrant of the diagram that matches this bulge. The transformations shown on the vertical and horizontal axes of this quadrant can help improve the fit between the variables.

Note that:

- There are multiple solutions. Some will fit better than others.
- sqrt and log make a value “smaller.”
- Raising to a power makes a value “bigger.”
- Each of these transformations equates to increasing or decreasing the scale of an axis.

Other goals in addition to linearity are possible, for example, making data appear more symmetric. Linearity allows us to fit lines to the transformed data.

Let’s revisit our dugongs example. The lengths and ages are plotted below:

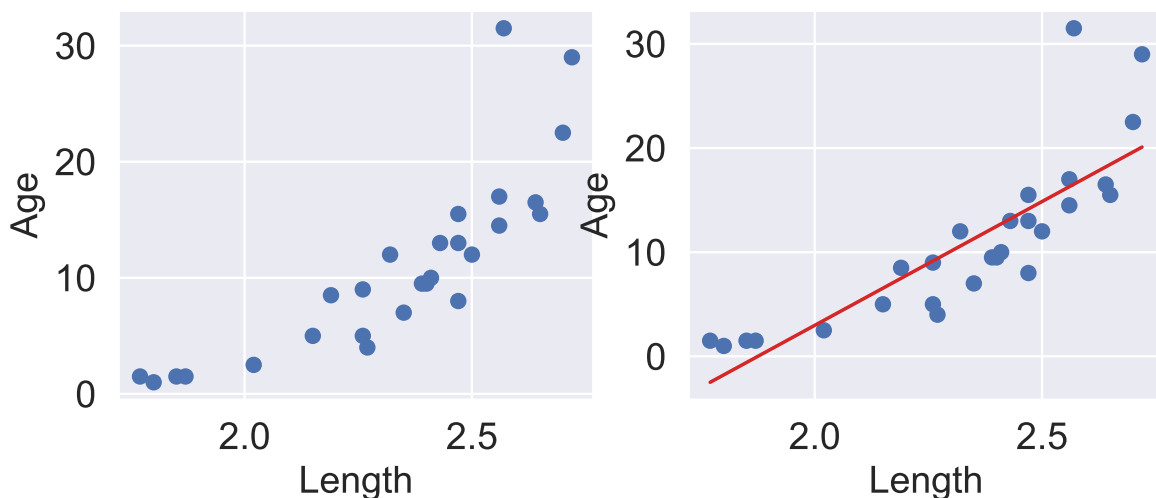
```

# `corrcoef` computes the correlation coefficient between two variables
# `std` finds the standard deviation
x = dugongs["Length"]
y = dugongs["Age"]
r = np.corrcoef(x, y)[0, 1]
theta_1 = r * np.std(y) / np.std(x)
theta_0 = np.mean(y) - theta_1 * np.mean(x)

fig, ax = plt.subplots(1, 2, dpi=200, figsize=(8, 3))
ax[0].scatter(x, y)
ax[0].set_xlabel("Length")
ax[0].set_ylabel("Age")

ax[1].scatter(x, y)
ax[1].plot(x, theta_0 + theta_1 * x, "tab:red")
ax[1].set_xlabel("Length")
ax[1].set_ylabel("Age");

```



Looking at the plot on the left, we see that there is a slight curvature to the data points. Plotting the SLR curve on the right results in a poor fit.

For SLR to perform well, we'd like there to be a rough linear trend relating "Age" and "Length". What is making the raw data deviate from a linear relationship? Notice that the data points with "Length" greater than 2.6 have disproportionately high values of "Age" relative to the rest of the data. If we could manipulate these data points to have lower "Age" values, we'd "shift" these points downwards and reduce the curvature in the data. Applying a logarithmic transformation to  $y_i$  (that is, taking  $\log(\text{"Age"})$ ) would achieve just that.

An important word on log: in Data 100 (and most upper-division STEM courses), log denotes the natural logarithm with base  $e$ . The base-10 logarithm, where relevant, is indicated by  $\log_{10}$ .

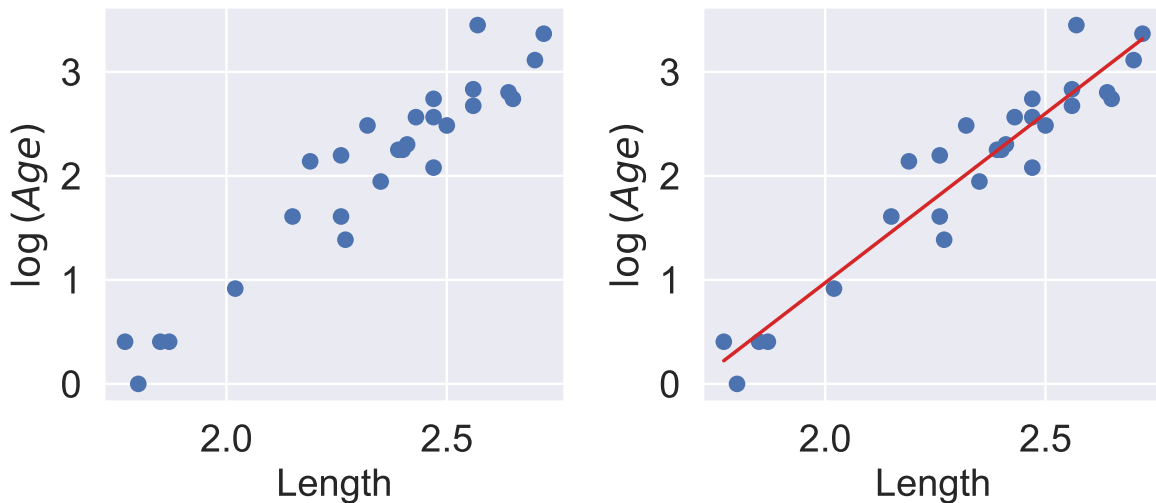
```
z = np.log(y)

r = np.corrcoef(x, z)[0, 1]
theta_1 = r * np.std(z) / np.std(x)
theta_0 = np.mean(z) - theta_1 * np.mean(x)

fig, ax = plt.subplots(1, 2, dpi=200, figsize=(8, 3))
ax[0].scatter(x, z)
ax[0].set_xlabel("Length")
ax[0].set_ylabel(r"$\log\{\text{Age}\}$")

ax[1].scatter(x, z)
ax[1].plot(x, theta_0 + theta_1 * x, "tab:red")
ax[1].set_xlabel("Length")
ax[1].set_ylabel(r"$\log\{\text{Age}\}$")

plt.subplots_adjust(wspace=0.3)
```



Our SLR fit looks a lot better! We now have a new target variable: the SLR model is now trying to predict the *log* of "Age", rather than the untransformed "Age". In other words, we are applying the transformation  $z_i = \log(y_i)$ . Notice that the resulting model is still **linear in the parameters**  $\theta = [\theta_0, \theta_1]$ . The SLR model becomes:

$$\hat{\log y} = \theta_0 + \theta_1 x$$

$$\hat{z} = \theta_0 + \theta_1 x$$

It turns out that this linearized relationship can help us understand the underlying relationship between  $x$  and  $y$ . If we rearrange the relationship above, we find:

$$\log(y) = \theta_0 + \theta_1 x$$

$$y = e^{\theta_0 + \theta_1 x}$$

$$y = (e^{\theta_0})e^{\theta_1 x}$$

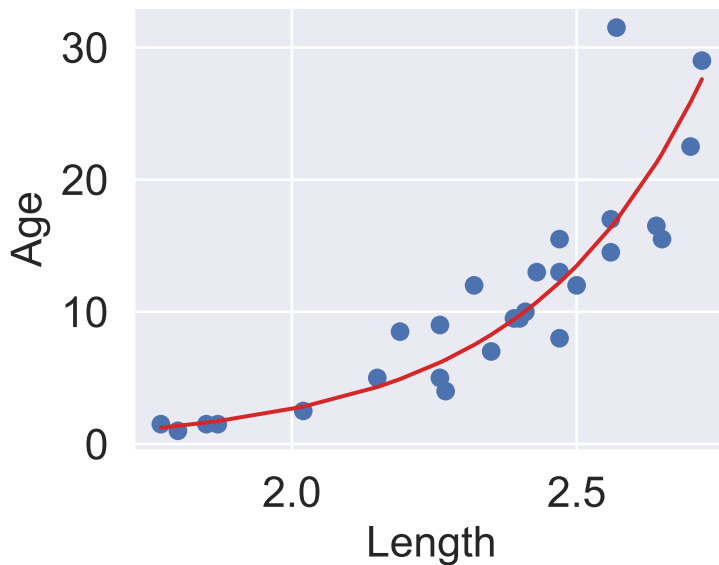
$$y_i = C e^{kx}$$

For some constants  $C$  and  $k$ .

$y$  is an *exponential* function of  $x$ . Applying an exponential fit to the untransformed variables corroborates this finding.

```
plt.figure(dpi=120, figsize=(4, 3))

plt.scatter(x, y)
plt.plot(x, np.exp(theta_0) * np.exp(theta_1 * x), "tab:red")
plt.xlabel("Length")
plt.ylabel("Age");
```



You may wonder: why did we choose to apply a log transformation specifically? Why not some other function to linearize the data?

Practically, many other mathematical operations that modify the relative scales of "Age" and "Length" could have worked here.

## 11.6 Multiple Linear Regression

Multiple linear regression is an extension of simple linear regression that adds additional features to the model. The multiple linear regression model takes the form:

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_p x_p$$

Our predicted value of  $y$ ,  $\hat{y}$ , is a linear combination of the single **observations** (features),  $x_i$ , and the parameters,  $\theta_i$ .

We'll dive deeper into Multiple Linear Regression in the next lecture.

## 11.7 Bonus: Calculating Constant Model MSE Using an Algebraic Trick

Earlier, we calculated the constant model MSE using calculus. It turns out that there is a much more elegant way of performing this same minimization algebraically, without using calculus at all.

In this calculation, we use the fact that the **sum of deviations from the mean is 0** or that  $\sum_{i=1}^n (y_i - \bar{y}) = 0$ .

Let's quickly walk through the proof for this: